Phase contrast in x-ray imaging

A thesis submitted for the degree of
Doctor of Philosophy

by

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for Lucy and Kalinda

Jan and Brian
“In every kind of magnitude there is a degree or sort to which our sense is proportioned, the perception and knowledge of which is of the greatest use to mankind. The same is the groundwork of philosophy; for, though all sorts and degrees are equally the object of philosophical speculation, yet it is from those which are proportioned to sense that a philosopher must set out in his inquiries, ascending or descending afterwards as his pursuits may require. He does well indeed to take his views from many points of sight, and supply the defects of sense by a well-regulated imagination; nor is he to be confined by any limit in space or time; but, as his knowledge of Nature is founded on the observation of sensible things, he must begin with these, and must often return to them to examine his progress by them. Here is his secure hold; and as he sets out from thence, so if he likewise trace not often his steps backwards with caution, he will be in hazard of losing his way in the labyrinths of Nature.”

— (MaC’laurin: An Account of Sir I. Newton’s Philosophical Discoveries. Written 1728; second edition, 1750; S( p. 18,19.)

The higher we soar on the wings of science, the worse our feet seem to get entangled in the wires

Unknown. (The New Yorker, 7 Feb., 1931)

Good judgment comes from experience; experience comes from bad judgment.

— Mark Twain
Declaration

I, Anthony Wayne Greaves, declare that this thesis entitled:

“Phase contrast in x-ray imaging”

is my own work and has not been submitted previously, in whole or in part, in respect of any other academic award.

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Dated this day, April 20, 2011
Abstract

X-ray phase contrast imaging (PCI) has the potential, over certain energy ranges, to improve conventional x-ray diagnostic practice by utilizing the higher phase than absorption coefficient in the complex index of refraction for low atomic Z materials, thereby potentially enhancing the differences between healthy and cancerous tissue. Mammography is a particularly suitable application due to its high biopsy incidence. Of the different types of PCI, the in-line holographic method or propagation-based imaging (PBI) has the ability to utilize polychromatic x-ray sources.

In clinical practice, polychromatic x-ray sources require filtering to remove the lower energy rays that have insufficient energy to penetrate the body and provide useful diagnostic information. However, the introduction of filters in PBI is known to cause phase contrast degradation, and this thesis examines both experimentally and theoretically, the various factors affecting phase contrast.

Experimental factors using a Feinfocus micro-focus, tungsten x-ray source with 0.5 mm beryllium inherent filtration, included: varying the tube voltage and source size, introducing extra filters of different materials and thicknesses including grain size and surface smoothness, and objects of different shapes and materials and at various positions in the beam. Image detection was via Fuji image plates and BAS-5000 scanner. The most convenient filter material was aluminium, and the object showing the best phase contrast was a thin walled, cylindrical fibre (Cuprophan RC55) normally used in dialysis. The x-ray spectrum of the tube was also measured using a
SiLi detector system, with and without various filters.

Theoretically, phase contrast was simulated via geometric ray optics, Fresnel and Fresnel-Kirchhoff wave diffraction methods. Inelastic scattering was also included in a simple model but was found to have only a very minor effect. Simulations showed good qualitative concurrence between the ray optics and Fresnel diffraction methods, with the Fresnel method providing greater detail in the line profile shape of the object, but essentially showing the same behaviour. Phase contrast reduction was found to be caused mainly by beam hardening, which narrows the phase peaks obtained from dispersion in the object, and together with source and detector considerations which then smooth the narrower filtered phase peaks more than the unfiltered case.

There were some discrepancies with theoretical simulations producing absolute values approximately twice that of experimental ones, but the overall behaviour of phase contrast with the imaging parameters was consistent.
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Chapter 1

Introduction

X-ray phase contrast imaging is a new technique that offers traditional diagnostic imaging, a new and complimentary way of imaging biological soft tissue. Since Röntgen’s discovery of x-rays in 1895, medical imaging practice has utilized the penetrative powers of x-rays to peer inside the human body. Röntgen’s rays (x-rays) were implemented in a combat situation as early as the Boer (1899-1902) war to search for bullets, shrapnel and bone fractures [1]. The underlying physical basis is the absorptive nature of the interaction of matter with electromagnetic x-ray radiation, which for example between bone or metal and soft tissue works particularly well, but not for small differences such as between cartilage, healthy tissue and early forms of cancer. The interaction of light or any electromagnetic radiation through matter can be described by the complex refractive index \( n = 1 - \delta + i\beta \), which contains the phase term, \( \delta \), as well as the absorption term, \( \beta \). The greater phase term, which has ironically, been ignored in medical imaging until recently, is up to three orders of magnitude greater than the absorption term, over the diagnostic energy range for low atomic Z materials such as breast tissue, as shown in Fig. 1.1.

Consequently, there is a greater x-ray phase change passing through soft tissue than absorption and hence the potential to image small differences in tissue density such as
lobular carcinoma [2]. To achieve this requires x-ray sources with high lateral coherence such as synchrotrons or the micro-focus tube, as used in this thesis, and appropriate geometry between source, patient and detector to allow these phase changes to interfere in a holographic sense and become apparent as a Fresnel diffraction fringe. However, as in the case of conventional x-ray tubes, the polychromatic micro-focus source must be filtered in the interest of patient safety. The beam filtration though, is known to interfere with the phase contrast process, and this along with other imaging parameters, is investigated in this thesis.

The thesis is constructed in three main parts. The first part from chapters 2-4 covers the literature in reference to origins of phase contrast, the image formation process and the interaction of x-rays with matter. At the end of chapter 4 (section 4.5.1), some minor original work is presented as a simple model of x-ray scattering from the sample and/or filter, as a possible mechanism interfering with phase contrast. The second and third parts contain the major original work. The second part, chapters 5-6, was experimental, and includes the search for a suitable test object by which to measure phase contrast and a novel software straightening program of the fibre images, to enable consistent measurements. The factors affecting phase contrast were then measured and quantified in chapter 6. The third part, chapters 7-8, contains the application of the
image formation process from chapter 3, with novel theoretical modelling procedures to enable calculation of the imaging process using Matlab\textsuperscript{TM} software. This analysis was able to separate out the various components of the imaging process to discern how filters harden the beam spectra, which in turn narrows the diffraction peaks that are smoothed out by source and detector considerations, more so than the unfiltered case. This unfortunately presents a problem for implementing phase contrast into clinical practice. The filters, which are necessary for patient health, also degrade the improvements phase contrast imaging brings to the images. It is shown further that this is a bulk effect, not dependent on surface properties or grain structure of the filter.

The details of the thesis construction are as follows.

1.1 Foundation

Beginning with the notion of phase, chapter 2 presents a historical introduction to phase contrast imaging, including Röntgen’s attempts to diffract x-rays and von Laue’s realization that the atomic spacing of crystals could diffract x-rays. Ever since then crystallographers have routinely applied the wave nature of x-rays to obtain information about the structure of materials, but its application to medical diagnosis has taken a century to achieve. This is due in part to the technical difficulties that x-rays present, in that sources with sufficient coherence were not developed until the 1950’s, and also in part to several great discoveries in other fields of study that had to be developed, namely Zenicke’s optical phase contrast microscope and Gabor’s idea of capturing electron phase information by inclusion of a reference wave which marked the beginning of holography. These developments are outlined in this chapter, including the three main methods of performing x-ray phase contrast imaging beginning with Bonse and Hart’s interferometry, to diffraction enhanced imaging and the in-line holographic method, which is the method used in this thesis. Applications such as phase retrieval and medical imaging particularly in regards to mammography are also included. Chapter 3
presents some history behind some of the methods used in the image formation process used in this thesis. Namely the geometric ray optical approach and the wave diffraction (non-crystallographic) formulation. The ray optical approach is presented because of its relative simplicity compared to the wave approach and its ease of implementation to use as a guide. The wave approach covers some history concerning the different formulations, of which the Fresnel and Fresnel-Kirchhoff methods were used in this thesis. Also included is a section on Fourier optics which is used extensively in the original work in chapter 8 to enable modelling of the test object in a numerically tractable form.

Chapter 4 examines the interaction of x-rays with matter and is mainly used to show how the complex index of refraction was derived from the classical theory of scattering. Absorption contrast is due to the combination of photoelectric, incoherent and coherent scattering processes, whereas phase contrast depends only on the coherent interaction. These topics are introduced before presenting the author’s own model of the scattering process is presented as a possible effect on phase contrast. Originally derived in a simpler form as part of a masters thesis [3], for the purpose of examining the magnitude scatter at a central point on a detector, it was extended and adapted across the entire detector, to determine the effect of incoherent scattering upon phase contrast imaging.

1.2 Experimental

The major original work starts in chapter 5, by first characterizing the system, and then determining the suitability of various test objects before settling upon the dialysis fibre used later in chapter 6. It also presents a novel method of straightening the images of the fibre containing non-uniformities, enabling consistency of phase contrast measurement, which worked well for reasonably straight sections. The simple scattering model from chapter 4 (section 4.5.1) was also tested, but was found to have very little
effect as the object and filter were very small and thin compared to the comparatively large imaging geometry.

Factors affecting phase contrast such as source size, tube potential, imaging geometry and filters are examined and measured in chapter 6. It is these measurements that are compared to the theoretical calculations in chapter 8. The beam spectra was initially simulated, but given the importance to this thesis, was also measured under different filtration conditions. These spectra measurements were incorporated into the simulations in chapters 7-8 for calculated profiles across the test objects.

1.3 Theoretical and simulations

Chapters 7-8 develop in detail the general image formation processes presented in chapter 3, for the case of an edge and a fibre for the purposes of simulation. For the case of the fibre (chapter 7), this required following the various angle changes of refraction of the geometric ray through the fibre and determining the energy intensity deposited on the image screen. Although the angle changes are in the order of micro radians, the geometry is such that small angle changes on the edges of the fibre, can lead to large changes at the image. The results were encouraging and gave similar intensity profiles to the experimental ones measured in chapter 6.

The heart of the thesis is contained in chapter 8, where the more accurate wave formulation was used to examine the image formation process. The Fresnel-Kirchhoff method was initially tried extensively before admitting failure, even though the image profiles were tantalizing close to experimental ones. There seemed to be a fundamental mismatch between the diffraction patterns and the background intensity. Rather than make ad-hoc assumptions to force the method to work, it was decided to use the less accurate Fresnel theory, which after some novel manipulation into a workable form, was able to give results in better agreement with the experiments. However, even though it was qualitatively correct under a variety of conditions, it systematically overestimated
the absolute values of phase contrast.

1.4 Discussion and Conclusion

Possible reasons for the discrepancy, such as the assumptions regarding the object and system properties are discussed in chapter 9. The conclusion of the thesis is given in chapter 10.
Chapter 2

Historical Introduction

This chapter traces the development of phase in visible light optics to its implementation as phase contrast in x-ray imaging. Unlike conventional x-ray absorption imaging which was utilized almost immediately from Röntgen’s discovery in 1895, the development of x-ray phase contrast took much longer to develop. This was, in part, due to the requirement for new types of sources such as synchrotrons which were developed in the 1950’s, and discoveries in electron microscopy of how to obtain the phase information from diffraction experiments. Thus x-ray phase imaging is the convergence of several discoveries over the past several decades plus many more incremental steps that can now be applied to an age old problem of better medical diagnosis. In this respect it becomes a complementary technique to the already refined technique of absorption imaging with the hope that it should lead to better diagnosis, with less patient dose.

2.1 Phase

The idea of light possessing the property of phase reaches as far back as to Thomas Young in 1804, who despite the authority of Sir Isaac Newton that light consisted
of particles, constructed a wave theory based upon the earlier ideas of Huygens and Grimaldi [4]. Using Newton’s own data with the correct path length differences between the slit and edges, together with Römer’s estimation of the speed of light, he was able to deduce both the frequency and wavelength of light. Furthermore, the wave is considered coherent if it has a well defined phase and hence the concept of phase became firmly established in the fields of optics and physics. Incidentally, it also played a crucial role in the development of quantum mechanics, where it may change by $2n\pi$ around any closed loop for a single valued, matter wave function. This was one of the arguments used by Niels Bohr to justify the quantization of electron orbitals which successfully quantified the hydrogen spectra in atomic theory [4].

When phase is used in reference to x-rays however, there are two distinct quantities of interest: (1) the phase of the incident radiation and (2) the real part of the refractive index decrement ($\delta$) of the medium, $n = 1 - \delta + i\beta$ (or $n = 1 - \delta - i\beta$ depending on convention for the incident plane wave $e^{\pm i(\omega t - kr)}$ [5]) [6]. For x-rays the refractive index (n), is less than unity, and furthermore the change of n with respect to wavelength ($\lambda$) $\frac{dn}{d\lambda}$ is greater than zero, corresponding to the realm of anomalous dispersion and the phase is advanced, unlike ordinary optical frequencies where $n$ is greater than unity and the phase is retarded. Although the absolute phase of the wave passing through the object is not directly measurable, the relative phase delay ($\phi$) to the reference wave is proportional to the optical path length through the medium which in turn is related to the real part of the refractive index

$$\phi(x, y; k) = -k \int_{-\infty}^{\infty} \delta(x, y, z'; k) dz'$$

(2.1)

where the phase $\phi$, in this equation, at any point $(x, y)$ on a screen, is a functional along the path of the real part of the refractive index through of the medium for some wave vector $k$. Interference with the reference wavefield causes the phase shift through the object to become apparent, even though the absolute phase of the wavefield is not apparent. Further extension of this to a partially coherent source, requires the time
average of the corresponding quantities for a fully coherent source which then become well defined and behave in a similar manner [7].

2.1.1 X-ray diffraction

“Ever since I began working on X-rays, I have repeatedly sought to obtain diffraction with these rays; several times, using narrow slits, I observed phenomena which looked very much like diffraction. But in each case a change of experimental conditions, undertaken for testing the correctness of the explanation, failed to confirm it, and in many cases I was able directly to show that the phenomena had arisen in an entirely different way than by diffraction. I have not succeeded to register a single experiment from which I could gain the conviction of the existence of diffraction of X-rays with a certainty which satisfies me.” – From W. C. Röntgen’s Third Communication, March 1897 [8]

Since non-crystallographic diffraction is used in this thesis, some brief history of x-ray diffraction is presented. Almost immediately after Wilhelm C. Röntgen’s (Fig. 2.1) discovery of x-rays in 1895, applications of imaging in various fields quickly developed, particularly medical imaging, which were based on the differential absorption of x-rays by materials. However, phase contrast imaging was not discovered via this route, as
it required knowledge of the wave properties of x-rays, which were developed by the pursuit of x-ray diffraction.

Although Röntgen discovered x-rays and vigorously pursued its properties, he was unable to demonstrate diffraction. Further attempts by Haga and Wind in 1903, using a fine slit, were not convincing enough to be widely accepted. Walter and Pohl were able to show diffraction effects in 1908 and 1909, using a tapering slit that was confirmed by P. P. Koch in 1910, who ironically was one of Röntgen’s assistants. This discovery enabled x-rays to be interpreted as being a wave phenomena together with the chance of deducing their wavelength from such an experiment. However, as is often the case when things appear easy, this was no simple feat because the intensity profiles as measured by Koch departed considerably from the equivalent optical case. It took the genius of Arnold Sommerfeld (Fig. 2.2a) in 1912 to develop a theory of diffraction formed by a deep slit, before analyzing the resultant curves of Walter, Pohl and Koch to conclude that the fuzziness of fringes was caused by the spectral wavelength range of the x-rays with the center occurring at around $4 \times 10^{-11}$ m [8].

So there was a conundrum for physicists at the end of 1911. There was strong
evidence of the corpuscular nature of x-rays from the photoelectric effect and an emerging indication of the wave nature of x-rays from diffraction effects. Then in 1912, Max von Laue (Fig. 2.2b) realized that the deduced wavelength of x-rays was roughly the same order as the atomic dimensions of various crystal structures and hence these could also be used to demonstrate diffraction phenomena. This led to the emergence of a the x-ray crystallographic community which paralleled the medical imaging community based upon the wave and the particle-like nature x-rays respectively. The conclusion of the wave nature of x-rays was extended further by William and Lawrence Bragg, father and son, who developed x-rays as a crystallographic tool for the analysis of various types of matter.

Some early successes of crystallography were the descriptions of simple structures such as rock salt (NaCl) and the concept of chemical bonding, which incidentally corroborated Niels Bohr’s atomic model from the analysis of x-ray intensities reflected from crystals. Later in the 1930’s, the structure of sterols, including cholesterol, were determined by Desmond Bernal and Dorothy Crowfoot Hodgkin. Over the next few decades, the structures of other biologically interesting molecules were discovered such as penicillin and vitamin B12 [8]. In 1953, Crick and Watson derived the now famous double helix structure of DNA from the work of Rosalind Franklin and Maurice Wilkins which marked a historical moment in science as the beginning of modern molecular biology [12]. This led Watson to deduce the helical nature of rod-like viruses and further work in 1956, by Watson and Crick and by Franklin and Aaron Klug produced a much deeper understanding of the general architecture of virus particles and showed that they were constructed of identical subunits packed together in a regular manner [13]. Similar analysis has also been applied to collagen and muscle structure which present the novel feature that the transform of an asymmetrical arrangement is not part of a space lattice. Patterns produced by regular materials such as crystals are easier to interpret, and although collagen and muscle have more disorder, they still produce a highly characteristic diffraction pattern [14]. More complex structures have been investigated by Kendrew and Perutz who sought the complete determination of the
proteins myoglobin and haemoglobin according to space-group symmetry, which have some 2500 atoms in the case of myoglobin and four times that number for haemoglobin [8]. More information on modern diffraction techniques can be found in Paris and Muller [15], Warren [16] and Kasai [17].

In summary, the wave-like properties of x-rays from initial slit diffraction experiments were confirmed via crystal diffraction which led in turn to utilization for the characterization of materials from simple structures to complex organic molecules. This process occurred in parallel to developments in medical imaging. The next section overviews the notion of phase contrast as developed in optical microscopy with its subsequent links to holography and coherence.

### 2.2 Phase contrast

Phase contrast was developed by Fritz Zernike (Fig. 2.3) in 1930, in a parallel to the discovery of x-rays by Röntgen in 1895. Zernike also used a black painted, darkened room to discover that there was another type of contrast different to the usual
absorption contrast. However unlike Röntgen who received immediate fame for his discovery, he was unfortunate in that his great discovery was overlooked at the world-famous Zeiss factories in Jena. Unlike previous studies such as Abbe’s and Kohler which had concentrated on absorption, Zernike looked into the formation of images of phase objects, which are defined as objects that are non-absorbing but influence the phase of the light transmitted by them. He realized that the diffraction pattern formed in the back focal plane of the objective of such objects differed characteristically from the pattern formed by absorbing objects. This led to the phase contrast method where phase annuli plates, arranged in a plane conjugate to the back focal plane of the objective and housed in a special tube, altered the beam in such a way that phase objects could be made visible. It was not until 1936 that the first prototype of a phase contrast microscope was developed at the Carl Zeiss corporation in Jena, as strangely, it was only when the German Wehrmacht (German ‘defense’ machine) took stock of all inventions which might serve in the war in 1941, that the first phase-contrast microscopes were manufactured.

2.2.1 Holography

The beginnings of holography date back to about 1920, from x-ray crystallography, where there was a goal to try to reconstruct a crystal structure from the x-ray diffraction pattern [19]. Since the pattern is considered as the modulus of the Fourier Transform squared, only the intensity information is available and the phase information is hidden. In the field of electron microscopy, 1927 saw the discovery of electron diffraction by Davison and Germer [20], and Thomson and Reid [21], which confirmed de Broglie’s matter wave hypothesis [4]. In 1943, Boersch noticed Fresnel fringes in an electron microscope showing the wavelike nature of the electrons and the realization that phase information was encoded into the fringes of the pattern [4]. The major breakthrough however, was pioneered by Dennis Gabor (Fig. 2.4) in 1948 [22], when he proposed the idea of holographic imaging, which was to capture this phase information by including
a reference wave. This idea was further extended in 1949 [24] and 1951 [25]. His motivation was to try to overcome the spatial resolution limits in electron microscopy caused by imperfect electron lenses [26], by means of determining the phase of the wavefront aberrations so as to deblur the images. Haine and Mulvey, in 1952 used a transmission type holographic method, that is now being widely employed in both modern x-ray and electron microscopy, that makes use of the fact that an out of focus image is an in-line-hologram [4], something that will be exploited in this thesis. X-ray holography was explored in the 1950’s by Baez [27] but the lack of high spatial coherence of x-rays prevented development for decades [28]. It has mainly continued in the realms of soft-x-ray microscopy due to powerful second and third generation synchrotron sources [29], [30]. In-line holography has continued around the “water window”, which are those photon energies around 0.3 to 0.5 keV (2.3-4.4nm) [31], which are important for both biological and materials imaging. The carbon K absorption edge is at 284 eV (4.4 nm), but water is transparent to soft x-ray radiation above 284 eV, whereas carbon atoms absorb this light [32]. The phase in this case is made visible by a reconstruction step which may be conceived as a method of phase retrieval [33]. A form of in-line holography [34] was developed earlier called microradiography or point
projection radiography and was applied to absorbing objects. However in this case, diffraction effects were considered as undesirable blurring of the image. The subsequent sections will show how in-line holography is related to x-ray phase contrast imaging.

2.2.2 Phase and coherence

Intimately connected to the concept of phase is the idea of coherence which is artificially divided into two forms, namely temporal and spatial coherence. Temporal coherence, sometimes called longitudinal coherence, refers to the finite bandwidth of the source, while spatial coherence or lateral coherence, refers to the finite extent of source in space [35]. Since the source used in this thesis is polychromatic, there is no temporal coherence. However, since the source is very small, in the order of about 4 µm, there is a high degree of spatial coherence and the following discussion begins with a discussion of full spatial coherence. Later in section 8.4.3, spatial coherence is included as convolution operation with the image profile determined via full coherence.

A coherent wave, is by definition, one with a well defined phase. Thus a spatially coherent wave is one in which two laterally displaced points on the same wavefront, possess the same phase. A wave or wavefield may be described by the complex quantity \( \Psi \) as

\[
\Psi = \left[ I(\mathbf{r}) \right]^{\frac{1}{2}} e^{i\phi(\mathbf{r})}
\]

where \( \mathbf{r} \) is the position in space of the wave, \( I(\mathbf{r}) \) is the intensity or equivalently the probability density of the wave, and \( \phi(\mathbf{r}) \) is the phase. The propagation of a wave in free space for a localized region can be described by \( \nabla \phi \), where surfaces of constant \( \phi \) can be visualized as wavefronts. For example, the phase distortion of a plane wave by a simple lens, results in a change in the direction of propagation of the wave, see Fig. 2.5. Since it is not possible to determine the phase directly, the phase change is evident by \( \nabla \phi \), which after propagation over a suitable distance, is revealed by changes in intensity.
One way to perceive the change in phase is by interferometry. Suitable combination of the wave of interest with a reference wave causes interference, from which the phase change may be deduced. Unfortunately one of the requirements of interferometry is coherence which is not well suited to x-ray imaging due to the relative experimental complexity [36]. By contrast, such high degree of coherence is not necessary for imaging, as for example in the case of optical microscopy, under certain conditions, optimum resolution occurs for partially coherent radiation [37]. Since Zernike, the technique of “defocusing” has been used for phase contrast imaging. This is equivalent to allowing the radiation to propagate a small distance to allow for changes in phase to create detectable intensity contrast. Conventional radiography places the detector as close as possible to the object for many applications, to minimize focal spot blurring. By increasing the distance between object and detector, and introducing sufficient source coherence, the phase properties of the object may be revealed. For example, Fig. 2.6 shows three cases of an image: (a) the raw phase object that absorbs minimal incident radiation and (b) the intensity distribution created a short distance downstream of the object. The third part (c) shows an interferogram of the same object.
2.3 X-ray phase contrast

X-ray phase contrast can be obtained in three different ways: (i), by interferometry, (ii), by crystal analyzer imaging and (iii) by in-line holography. The first and third methods use the interference between scattered wavefronts from the sample with a reference wave. Examples are multi-energy holography (MEXH) [38], [39], [40] and phase contrast imaging (PCI) [41], [2], [42]. The second method utilizes a selective measure of the reflective properties of a crystal analyzer to separate the angular distribution of refracted beams from the object and is often termed diffraction enhanced imaging (DEI) [43]. The third method is also known as phase propagation imaging (PPI) [44] (or phase based imaging (PBI) [45]).

2.3.1 Interferometry

Interferometric methods were first applied by Bonse and Hart and the first phase image of a non-crystalline object was formed in 1965 based on a triple-Laue-case (LLL) interferometer, one of the most commonly used x-ray interferometers [46], which is usually constructed from one monolithic crystal [47] and consists of three parallel lamellas [48]. The first lamella, called the splitter, divides the incident beam into a transmitted and reflected beam. The second lamella, the mirror, divides the beams once again and two of the beams are redirected towards one another where they interfere at the third lamella, called the analyzer crystal. Originally this type of device was
used to detect lattice deformations in the analyzer crystal. The intersection of the beams form a standing wave with a period equal to the crystal lattice of the first two blocks. Imperfections in the third crystal, such as rotational stress, cause differences in the nodes of the standing wave and will show itself as a Moirè pattern as black and white stripes. For imaging, a perfect analyzer crystal is used and an inhomogeneous object is placed on one of the paths to cause a phase shift. For a simple object such as a wedge, which is homogeneous, interference fringes of equal thickness and equal distances between them are observed. Such a method may be associated directly with the phase shift $\phi$ [49]. Further work in this area can be found in Momose [50], [51], [52].

### 2.3.2 Diffraction Enhanced Imaging

The basis of diffraction enhanced imaging (DEI) is refraction [43]. When an x-ray crosses a boundary between two materials of different refractive index say $n_1$ and $n_2$ according to Snell’s law, the ray is deviated. For curved surfaces such as spherical or cylindrical shapes, diverging x-rays from the source will be incident over a range of angles from 0 to $90^0$. For typical $\delta$ values in the order of $10^{-6}$, these deviations can be in the range of 0 to $10^{-3}$ radians, since the critical angle of refraction is roughly $\sqrt{\delta}$. At the boundary of such an object, refraction forms a Fresnel zone to the detector and the experimental arrangement of DEI consists of a collimator and analyzer which was pioneered by Forster et al in 1980 [53]. It differs from interferometric methods by measuring not the phase but the phase gradient $\nabla \phi$ [49]. Applications to biological materials were studied by Somenkov and Shil’shtein in 1991 using scattered radiation analyzed by Bragg diffraction from a Silicon (333) symmetrical reflection for both the incident beam and analyzer, and the image was recorded on film by scanning the object with a slit [54].

The contrast mechanism is due to slight deviations of the beam caused by refraction with the object. These rays are in turn discriminated by the analyzer screen. Sensitivity of this technique is due to the degree of slope of the reflection curve and maximum
contrast occurs on the edge of the reflectivity maximum. Consequently this method is able to measure $\nabla \phi$, the differential of the phase of the object perpendicular to the wavefront.

Ingal and Beliaevskaya imaged non-crystalline objects using Laue diffraction (transmission) for the analyzer crystal [55]. An illustration of the apparatus is shown in Fig. 2.7 and of the results in Fig. 2.8.

Figure 2.7: Experimental geometry of Ingal and Beliaevskaya using Laue diffraction for the crystal analyzer

The incident beam is monochromatized by two asymmetrical Bragg diffraction crystals and this configuration allows simultaneous imaging of the reflected and transmitted beam. The images were named Phase Dispersion Images (PDI) by the authors and the contrast can be split between “area contrast”, and “boundary contrast”. More detail about the mechanism of contrast will be given in Chapter 3.

One of the benefits of such a technique is the added value of incoherent (Compton) scatter rejection which plagues conventional radiography. Scatter rejection devices, often called anti scatter grids, and/or air gaps are used to try and prevent this type of radiation from reaching the detector where it adds noise to the image, but in the case of anti-scatter grids, have significant disadvantages such as only partial rejection of scatter with a correspondingly significant increase of dose to the patient. In this
Figure 2.8: X-ray images of a fish by Ingal and Beliaevskaya (a) absorption image made with Mo radiation (b) phase dispersion image (pdi) [55]

In this case, the rocking curve of the analyzer crystal can be used to select which interactions of the x-rays with the sample are to be displayed by micro-radian adjustment of the crystal, which means only those that satisfy the Bragg condition will be reflected, since the window of acceptance is very small. Incoherently scattered x-rays can be made to fall outside this window and therefore be rejected. The image closely resembles an ordinary radiograph with excellent scatter rejection.

### 2.3.3 In Line Holography

The holographic approach is to allow the weakly interacted part of the x-ray beam, which picks up information about the object by a change of phase, to combine with the main part of the beam, in the same direction, in-line to the detector. The main beam becomes the reference beam, and the two combine to form an interference pattern. The in-line holographic approach developed for x-rays can be achieved by two methods, the monochromatic and polychromatic approach. The theory behind in-line holography has been developed by Gureyev [41], [56], [57] and others [6], and is based on the idea that a pure phase object produces an inhomogeneous phase shift which transforms
into an intensity distribution at a certain distance from the object. This method produces an intensity proportional the Laplacian of the phase, expressed as $\nabla^2 \phi$ and the intensity distribution may be represented by an approximation of the transport of intensity equation (TIE) \[58\]. This can be obtained from the solution, $E(\mathbf{r})$, to

$$[-\nabla^2 - K^2]E(\mathbf{r}) = K^2 \chi(\mathbf{r})E(\mathbf{r})$$ \tag{2.3}$$

where $K = \omega/c$, and $\chi(\mathbf{r})$ is the complex susceptibility as a function of position $\mathbf{r}$. The solution $E(\mathbf{r})$ may be written as a scalar wave field,

$$E(x, y, z) = I^{1/2}(x, y, z)e^{ikz+i\phi(x,y,z)}$$ \tag{2.4}$$

where $k=2\pi/\lambda$ is the wave number, $E$ is now the amplitude, $I$ is the intensity and $\phi(x,y,z)$ is the phase shift \[49\]. For use with the TIE, under conditions of validity, both the intensity and the phase shift are assumed to be slowly varying functions of position $(x, y, z)$. Under these conditions and the weak absorption approximation, Gureyev \[57\] gives the TIE for the case of an incident plane wave as

$$k \frac{\partial I(x, y, z)}{\partial z} \approx -\nabla_{\perp} \cdot [I(x, y, z)\nabla_{\perp} \phi(x, y, z)] \tag{2.5}$$

$$\simeq I_0(x, y, z)\nabla_{\perp}^2 \phi(x, y, z) + \frac{\nabla_{\perp} I(x, y, z) \cdot \nabla_{\perp} \phi(x, y, z)}{\text{cross term} \simeq 0}$$

$$\Rightarrow k \frac{\partial I(x, y, z)}{I_0 \partial z} = \nabla_{\perp}^2 \phi(x, y, z)$$

where

$$\nabla_{\perp} = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y})$$ \tag{2.6}$$

and the partial derivative on left hand side of Eq. 2.5 may be approximated by a difference equation for phase retrieval applications as explained in section 2.4.1

$$\frac{k}{I_0} \frac{I_z - I_0}{\Delta z} \simeq \nabla_{\perp}^2 \phi$$ \tag{2.7}$$
Thus the intensity distribution from $I_0$, where $z = 0$, to a distance $z$, denoted as $I_z$, is proportional to $\nabla^2_\perp \phi$.

One consequence of the holographic approach is that this type of phase contrast image is dependent on the distance from the object to the detector. At small distances only the absorption image is apparent. Increasing the detector distance allows the formation of a Fresnel type fringe between parts of the object with differing phase shifts. This is the main advantage of the technique, in that visually it allows for excellent definition, far better than the absorption type images that have characterized conventional radiography until recently. At further distances, more Fresnel type fringes can be seen which degrade the image. Thus there is an optimum distance to be sought, which is part of the topic in this thesis. Furthermore, unlike interferometry, this effect is not considered parasitic, nor does it require complex reconstruction techniques such as the Transport of Intensity Equation (Eq. 2.5) for phase retrieval, and the interference fringe actually emphasizes the edges between parts of the object with differing phase and this increases the contrast and resolution of the image.

There are however, some problems associated with this type of imaging. In order for phase contrast of this nature to be readily seen, it is necessary to have high source coherence as used in interferometry. But this is not the only factor to be considered. All parts contributing to the beam formation must be taken into account such as filters, collimators, monochromators etc. All have a part to play in the final beam coherence and the subsequent effect on the resulting image. For example, artifacts from the beryllium filter window on the beam line can be seen clearly superimposed on images by various researchers such as Carlsson et al [59] and Cloetens et al [60].

**Monochromatic Source**

An example of the monochromatic approach, is by Snigirev et al [61] at the European Synchrotron Research Facility (ESRF) Optics beamline who had an experimental setup
shown in Fig 2.9.

![Experimental geometry of Snigirev et al for in line holography](image)

Figure 2.9: Experimental geometry of Snigirev et al for in line holography

The monochromator selects the wavelength used to perform the imaging, which for synchrotron sources there is so much available flux that this causes no problems. In this approach, an inhomogeneous object causes phase shifts in the beam that can be detected as intensity variations as long as the distance between the object and the detector is sufficient, i.e. in the Fresnel region. This is seen as a measurement of $\nabla^2 \phi$.

It differs from the previous diffraction based approach in that there is no analyzer crystal which is unnecessary since the resolution of the crystal is limited by extinction and the narrow angular acceptance would cut off the diffraction pattern [61].

**Polychromatic source**

The polychromatic approach by Pfeiffer et al [62] and Wilkins et al [63] is another extension of in-line holography. Rather than selecting one wavelength, all wavelengths of the available spectrum are used.

X-rays traversing an object will vary according to the local refractive index properties. Using the geometrical optics approximation, the phase difference for a ray path through the object relative to one travelling through a vacuum is given by
Eq. 2.1, which away from absorption edges becomes

$$\phi(x, y; z, k) = -\frac{2\pi r_e}{k} \int_{-\infty}^{z} \rho(x, y, z') \, dz'$$

(2.8)

where the optical axis is along $z$, $k = \frac{2\pi}{\lambda}$, $r_e$ is the classical electron radius, and $\rho$ is the electron density of the object [63]. The refractive index for x-rays is $n = 1 - \delta + i\beta$, which is wavelength and material dependent. For light atomic number materials over the 10-100 keV range for example, $\delta$ is the order of $10^{-5}$ or $10^{-6}$, differing slightly for each wavelength. The phase of the wavefront is taken to be $kz - \phi$, corresponding to a phase advance for $\phi < 0$. The gradient of the phase perpendicular to the incident wavevector, determines the direction of the local propagation vector $s$, and can be written in the paraxial approximation as

$$s(x, y, z) \approx \left( -\frac{\delta \phi}{\delta x}, -\frac{\delta \phi}{\delta y}, k \right)$$

(2.9)

where $|\nabla_{\perp}\phi| \ll k$, so that $s(x, y, z)$ is normal to the wavefront at the point $(x, y, z)$. The angular deviation of the normal to the wavefront, $\Delta\alpha$, can be expressed as

$$\Delta\alpha \approx \frac{1}{k} |\nabla_{\perp}\phi(x, y, z)| = \left| \nabla_{\perp} \int_{-\infty}^{z} [\delta(x, y, z')] \, dz' \right|$$

(2.10)

and is thus dependent on the projected variation of the refractive index perpendicular to the propagation vector, $k$.

This approach is attractive due to its comparative simplicity compared to crystal based approaches and its similarity to conventional radiography. Utilizing the polychromatic spectrum makes good use of the photon flux of the source if it is not a synchrotron source, as for example a microfocus source, see Fig. 2.10. The use of a microfocus source has an advantage of having a divergent x-ray beam that is useful for magnification. As a consequence this technique is readily adaptable to clinical practice [64]. One of the reasons for using such a source is it having a high degree of spatial coherence. The effect of source size on image quality was explored by Pogany
2.4 Some Applications

There are some important applications of phase contrast that are relevant to this thesis, namely phase retrieval and medical applications. The phase retrieval is peripheral to this thesis but well worth mentioning as currently there is much endeavour to determine the phase information inherent in not just x-ray images, but related areas such as optical and electron microscopy. Directly related to this thesis are the medical applications and these are motivating factors for examining the effect of filters, which are important.
for limiting patient dose.

2.4.1 Phase Retrieval

Current detectors used in imaging for optical and higher frequencies are not sensitive enough to the phase disturbance of a complex electromagnetic wave in passing through an object [37]. The field of phase retrieval seeks to determine the phase information from intensity measurements by using phases obtained through virtual optics in image processing software to form an extension of the optical system [66]. This powerful technique would enable total knowledge of the system regardless of whether or not the system was realizable in hardware. All possible modes of microscopy could then be emulated, and physically difficult or expensive devices such as mirrors or beam splitters may be realized in software instead of hardware, such as in coherent X-ray and atom imaging.

For example, in the field of electron microscopy, most objects of interest show almost entirely phase information, hence there are at least three areas of interest where phase retrieval is desired. Since the phase information is lost upon recording of the intensity image, methods of overcoming this problem must be found.

The most well known method is the one developed in 1972 by Gerchberg and Saxton [67]. The intensity image and the far-field(Fraunhofer) diffraction pattern are used as inputs to this iterative type method. An initial guess is made of the phase and Fourier transformed with the intensity pattern and then the result compared to the Fraunhofer pattern. The measured intensity of the diffraction pattern is then substituted for the calculated pattern and a reverse transform is performed to provide a refined estimate of the phase distribution. This again is repeated using each time the refined estimate until the a solution converges to its correct value. Variations of this technique were implemented by Fienup [68] and Miao et al [69].

As mentioned previously, the defocus methods used in optical and electron
microscopy use the idea of a pure phase object as being described by the Laplacian of the phase \( \nabla^2 \phi \) [58]. This is related to adaptive optics used in astronomy to correct for distortions created by turbulence in the atmosphere such as the curvature sensing technique by Francois Roddier et al in 1988 [70]. In this case the defocus method is used to give quantitative information about the distortion which can be corrected by the adaptive optics.

In the area of x-ray imaging and the advent of synchrotron sources, particularly third generation sources that have a high level of spatial coherence, imperfections in the beam optics and windows can produce intensity modulations at the detector [71]. The types of phase retrieval methods that aim to overcome this problem has been summarized by Nugent [71] and a brief description of these methods will be given here. The approaches can be divided into direct and indirect or iterative methods. Of the direct approach, there are at least five different methods: Guigay’s method [72], transport of intensity approach [73], multi-wavelength approach by Gureyev et al [41], homogeneous sample approach [74] and phase-only approach [75]. These methods generally use two independent data sets to provide a plane of information for the real and imaginary parts of the object. Guigay’s method is to use two planes displaced fairly widely apart and known spacing and the object is assumed to only weakly interact with the incoming radiation. The transport of intensity equation approach by contrast uses two planes that are only a differential apart. The method is reliable with a unique solution as long as the intensity is positive. The multi-wavelength approach assumes that the optical properties of the sample are wavelength independent and that a small change in wavelength can have a similar effect to a small change in propagation distance. The homogenous sample approach assumes that the object consists of a single material with known composition. In this approach only one intensity data set is required with the assumption that the interaction of the sample and field is sufficiently weak to linearize the appropriate equations. The phase-only approach uses data taken from a short distance of the object with the assumption that absorption can be neglected. All these approaches have relative merits in regards to uniqueness, stability and noise and
are described more fully in Nugent [71].

The other approach is the indirect or iterative type approach which is often used when analytical relationship between the wave-field and measurement causes invertibility problems. Indirect methods have the advantage of allowing \textit{a priori} information to be included, as well as experimental uncertainties such as noise. This type of approach may be further subdivided into multiple-intensity measurements and far-field methods. The multiple-intensity measurements originated in the field of electron microscopy (see Coene et al [76]). Intensity measurements from a range of distances along the optic axis are taken and then using the laws of optical propagation, the method attempts to find a complex wave that is consistent with all of the measured data. Since there are numerous intensity measurements, the phase recovery is very robust although the solution is not necessarily unique, but it is stable with respect to noise. The far-field methods can be further subdivided into another five variations. The most well known is the Gerchberg-Saxton algorithm as mentioned earlier [67]. This method uses a measurement taken in one plane in the far-field regime and another in the plane of interest to be recovered. The phase is initially guessed and then Fourier transformed into the corresponding diffraction pattern at the far-field and altered according to the measured pattern. Due to the requirements of high resolution images, it has not found widespread application. A second variation of this, called the Gerchberg-Saxton-Fienup algorithm, uses only a single far-field image plus some \textit{a priori} information about the shape of the scattering object. It has been shown to be almost unique by Bates to within some very rare conditions of no practical importance [71]. This approach has been continued by a number of workers in the field such as Miao [77], Robinson [78], Chapman [79], [80]. A third variation of this approach called the Gerchberg-Saxton-Fienup in the Fresnel region is similar except that it utilizes the Fresnel region has been used by Nugent at al [81]. The fourth variation is called Ptychography, which uses multiple diffraction patterns obtained by scanning localized illumination of a specimen [82]. The sample or beam is displaced while recording the image at each displacement. The multiple data is then assembled
into a single image usually by iterative methods. The fifth variation is called astigmatic
diffraction which controls the phase structure of the illuminating wave as a way of
determining the phase of the detected wave. This has been utilized by Nugent et al [81],
produces a unique solution but at the price of increased experimental complexity [71].

2.4.2 Medical Applications

The practical aspects of phase contrast enhanced imaging is an issue involving at least
two objectives which can be cast in terms of image quality and patient dose. Clearly for
widespread use of the technique, a practical source with high coherence must be found
which rules out synchrotrons. The use of gratings has been put forward by Pfeiffer et
al [62] and coded apertures by Olivio and Speller [83]. An alternative is a microfocus
source as put forward by Wilkins et al [63]. This issue will be explored shortly. The
other main issue is patient dose which is one of the great advantages offered by phase-
contrast imaging. When imaging human or animal specimens, soft x-rays less than
around 15 keV must be filtered out as they are absorbed by the skin and subcutaneous
tissue and contribute little diagnostic information [84]. Energies higher than 50 keV
undergo multiple scattering, which reduces the signal to noise ratio (SNR) and are less
useful for imaging. Therefore there exists an x-ray window of approximately 15-50 keV
for imaging biological specimens.

One medical application suitable for PBI is mammography (14-30 keV), due to its
high biopsy incidence. Inaccuracies are due to reproducibility of breast compression,
limitation of film screen combinations and the difficulty of perception for the radiologist
of pathological structures. Cancers for example, seem to have a higher effective atomic
number than ordinary tissue and hence a higher linear attenuation (10%) [84]. However,
if these are small or next to regions of lower attenuation but of longer x-ray path length,
then the subsequent absorption contrast may be imperceptible see Figs. 2.11 and 2.12.
To make absorption effects more readily perceptible, chemical contrast agents are often employed. This is a common procedure in angiography where iodine based contrast agents are injected to make blood vessels and other structures such as the heart, more readily visible. These often involve some risk to the patient and have to be carefully administered.

An alternative to using chemical contrast agents may be the use of acoustic modulation. The use of ultrasonic pressure to exert force on an object that displaces internal parts by tens to hundreds of microns, allows a type of ‘contrast agent’ that highlights the high frequency features. For more information see Hamilton [86].


2.5 Summary

The historical development of the applications of x-rays has followed an “interferometric” type split along the wave-particle duality very early since their discovery. The imaging community has developed absorption techniques based on the particle-like nature of x-rays while the crystallographic community has developed diffraction techniques based upon the wave-like nature. Through developments in optical phase contrast and electron microscopy, the techniques of Zernike and Gabor have only relatively recently been applied to x-ray phase contrast using sources with good lateral coherence.

Conventional mammography according to Fitzgerald [87], has a high rate of false positives and negatives, with 10-20% of women with palpable abnormalities not being detected. This is the limitation of conventional absorption based radiography and
provides the driving need to improve breast cancer detection technology. The use of x-ray phase contrast techniques provide the promise of greater soft tissue differentiation but are still in progress towards clinical implementation.

This chapter has traced the origins of the concept of phase to the development of the background of the three principal methods of x-ray phase contrast imaging, namely interferometry, DEI and PBI. All these have potential applications for medicine and biology, and measure respectively the phase $\phi$, gradient of phase $\nabla \phi$ and Laplacian of the phase $\nabla^2 \phi$. They have the extra requirement of sources with good spatial coherence or effective source size and sufficient distance to the detector to allow the wave-like nature of x-rays to show interference contrast as well as absorption contrast. Sources such as synchrotrons provide excellent coherence and flux but are not so practical for clinical practice. The PBI method however using microfocus tubes may offer a potentially feasible method as long as sufficient spatial coherence is maintained with adequate beam filtration to limit patient dose.
Chapter 3

Phase contrast theory

This chapter presents an outline of the theory of phase contrast formation in the x-ray regime from two perspectives, namely the geometric ray theory and wave diffraction. As a first approximation, image formation may be conceptualized as a deviation of wave fronts propagating to the image screen, as described by the geometric ray theory. This method, using refraction rather than diffraction, has the advantage of simpler implementation and is likely to show the gross structure of the image giving an idea of the image formation process without the fine detail as expected from diffraction theory.

Next the diffraction approach is outlined, based on the principles of Huygens, Young, Fresnel and Kirchhoff. Using the superposition of waves, it is able to explain a wider class of phenomena but unfortunately is harder to implement due to the highly oscillatory nature of the integrand. It has been successively used in various forms, by many researchers in the field to calculate expected image formation for simple objects such as slits, apertures, edges, spheres and cylinders. It has been used this in thesis to verify the ray optics theory of image formation of a hollow cylindrical object.

This chapter is intended to be an outline of some of the methods used in the literature as a basis and comparison to the ones used in this thesis. Chapter 7 details the ray tracing method and chapter 8 details the diffraction approach.
3.1 Ray tracing and geometric optics

There are two fundamental approaches involved in ray tracing. The simplest approach to image formation in the presence of an object, based on heuristic geometrical principles, is called the geometric ray theory. In this case, refraction at the boundary of an object causes the rays to deviate, according to Snell’s theory of refraction and Fermat’s principle of least time. Historically these principles were generalized by Euler, Lagrange, Jacobi and Hamilton into an extensive mathematical theory. This chapter will present a method for calculating image formation based on these principles.

The second approach, begun in 1953 by Joseph Keller is called the Geometric Theory of Diffraction (GTD) [88]. This gave rise to the asymptotic expansion which extended the ray theory to explain a wider range of wave phenomenon to include such things as calculation of amplitudes and polarization particularly within anisotropic analysis, and diffracted rays. This approach, however will not be followed here as instead, image formation based on wave diffraction will be pursued.

Starting at either the wave equation or Maxwell’s equations, the eikonal equation may be derived which describes the relationship between the optical path \( S(\mathbf{r}) \), called the eikonal (Greek word meaning image), and the refractive index \( n(x, y, z) = \sqrt{\varepsilon_r \mu_r} \) [89].

\[
(\nabla S)^2 = n^2
\] (3.1)

The level surfaces of \( S(\mathbf{r}) \), i.e. when \( S(\mathbf{r}) = \text{constant} \), represent geometrical wave fronts of constant phase [37]. For homogeneous media the paths of the rays are straight lines, but for inhomogeneous media they are curved. Thus rays can either represent the direct path of light or the direction normal to the wave surfaces \( S(\mathbf{r}) \). This formulation is similar to an electrostatic potential, describing the equipotential surfaces that are everywhere normal to the fields. The eikonal is considered to be the basis of ray optics from which Fermat’s principle may be derived or vice versa [90].
The normals to these surfaces are given by \( \nabla S = n \hat{s} \), where \( \hat{s} \) is a unit vector normal to the wavefronts and tangent to the light ray. If the wavefront can be written in the form

\[
\psi(\xi, \eta) = B(\xi, \eta)e^{i[kz - \phi(\xi, \eta)]}
\]  

(3.2)

where \( B(\xi, \eta) \) is the amplitude function and the eikonal is written as \( S(\mathbf{r}) = kz - \phi(\xi, \eta) \), representing the path of the ray with phase \( \phi \), then \( \phi < 0 \) corresponds to a phase advance compared to ordinary optics, for those parts of the wave undergoing distortion by an object. In the paraxial approximation, the propagation vector \( \mathbf{s}(\xi, \eta, z) \) can be written as [63]

\[
\mathbf{s}(\xi, \eta, z) \approx \left( -\frac{\partial \phi}{\partial \xi}, -\frac{\partial \phi}{\partial \eta}, k \right)
\]  

(3.3)

since \( S(\mathbf{r}) = kz - \phi(\xi, \eta) \) then \( \nabla S(\mathbf{r}) = -\frac{\partial \phi}{\partial \xi} \hat{\xi} - \frac{\partial \phi}{\partial \eta} \hat{\eta} + k \hat{z} \)

where it is assumed \( \nabla \perp \phi \ll k \) and \( \hat{s} \) is normal to the wavefront at the point \( (\xi, \eta, z) \). Variations in refractive index \( n \) and path length through an object lead to changes in phase \( \phi \), of the wavefront.

As an example consider a general two dimensional image cross section of an object with parameters as shown in Fig. 3.1, and follow the derivation as developed by Peterzol et al [91]. The object is located at some distance along the optic axis, where the object plane \( (\xi, \eta) \) is chosen to cross at some location along \( z \) within the object at a distance \( r_s \) from the source. The image plane \( (x, y) \) is located further down the optic axis \( z \) at a distance \( r_d \). Rays from the source are refracted by the object to land at some point on the image plane. There is the assumption of a one-to-one correspondence between points on the projection of object on to an exit plane and points in the image.

The angular deviation of the ray \( \mathbf{s} \) can be expressed as

\[
\alpha \approx \frac{1}{k} |\nabla_{\xi, \eta} \phi(\xi, \eta, z)| = \left| \nabla_{\xi, \eta} \int_{-\infty}^{z} [\delta(\xi, \eta, z')]dz' \right|
\]  

(3.4)
where $\phi$ the phase, and $\delta$ the refractive index decrement, are related as in Eq. 2.1. This shows that the angular deviation is proportional to the projected electron density (Eq. 2.8) in the direction perpendicular to the wavevector $k$ [42]. For light atomic materials, x-rays of the order of energies between 15-30 keV are deviated by a few tens of microradians [91]. The next section describes how the geometric optics approach can be used to calculate an approximate intensity redistribution of these deviated rays.

### 3.1.1 Projection to a screen and the Jacobian

If the incident rays are considered to propagate parallel to the $z$ axis for the moment, and to interact with the object located at the axis $(\xi, \eta, r_s)$, with the dimensions of the
CHAPTER 3. PHASE CONTRAST THEORY

object small compared to the distance to the screen, then the incident intensity can be denoted by \( I(\xi, \eta) = I_0 \). As a consequence of angular deviation by the object, the ray position on an image screen located at \((x, y, r_d)\) can be written as

\[
\begin{align*}
x & \approx \xi + r_d \alpha_\xi(\xi, \eta) \\
y & \approx \eta + r_d \alpha_\eta(\xi, \eta)
\end{align*}
\] (3.5)

where \( \alpha_\xi \) and \( \alpha_\eta \) represent the projections of the deviation angle \( \alpha \) at the image screen, and, for a given vacuum wavelength \( \lambda \), are defined as

\[
\begin{align*}
\alpha_\xi & \approx \frac{\lambda}{2\pi} \frac{\partial \phi(\xi, \eta)}{\partial \xi} \\
\alpha_\eta & \approx \frac{\lambda}{2\pi} \frac{\partial \phi(\xi, \eta)}{\partial \eta}
\end{align*}
\] (3.6)

The intensity on the screen is related to the intensity at the object by the Jacobian, \( J \), via

\[
I(x, y) = I(\xi, \eta)J
\] (3.7)

where

\[
J = \left| \frac{\partial (x, y)}{\partial (\xi, \eta)} \right|^{-1}
= \begin{vmatrix}
1 + r_d \frac{\partial \alpha_\xi}{\partial \xi} & r_d \frac{\partial \alpha_\xi}{\partial \eta} \\
r_d \frac{\partial \alpha_\eta}{\partial \xi} & 1 + r_d \frac{\partial \alpha_\eta}{\partial \eta}
\end{vmatrix}^{-1}
\approx \left[ 1 + \frac{r_d \lambda}{2\pi} \nabla^2 \phi(\xi, \eta) \right]^{-1}
\] (3.8)

The approximation is obtained by ignoring the products of the partial derivatives since they involve terms with factors \((r_d \lambda/2\pi)^2\) and \(r_d \lambda \ll 1\). Furthermore, if
$\frac{r_d \lambda}{2\pi} \nabla^2 \phi(\xi, \eta) << 1$, this can be simplified to

$$I(x, y; \lambda) \approx I_0 \left[ 1 - \frac{r_d \lambda}{2\pi} \nabla^2 \phi(\xi, \eta; \lambda) \right]$$

(3.9)

where $I_0 = I(\xi, \eta)$. This now gives the intensity arriving at the image screen as a function of the incident intensity upon the object, modified by the Laplacian of the phase upon its passage through the object.

The assumption of the incident rays being parallel to the z axis may be relaxed and allow for the more general point source, located at a distance $r_s$ from the object. The magnification factor $M$ is

$$M = \frac{r_s + r_d}{r_s}$$

(3.10)

which modifies the equation of the rays to

$$x \approx M\xi + r_d \alpha_\xi(\xi, \eta)$$

$$y \approx M\eta + r_d \alpha_\eta(\xi, \eta)$$

(3.11)

Now the Jacobian is modified, resulting in the the beam intensity as

$$I(x, y; M; \lambda) \approx \frac{I_0}{M^2} \left[ 1 - \frac{r_d \lambda}{2\pi M} \nabla^2 \phi(\xi, \eta; \lambda) \right]$$

(3.12)

This expression has been derived by many others such as Wilkins et al [63], Pogany et al [65], Cloetens et al [60] etc, and forms the basis of calculating image formation based on geometric optics. It shows that phase contrast varies with the distance between the object and screen $r_d$, the wavelength $\lambda$ and the variation in phase across the object $\nabla^2 \phi$. Attenuation in the object can be described by including the absorption via the Bouger-Beer-Lambert law

$$I(x, y; M; \lambda) \approx \frac{I_0 e^{-2\mu(\xi, \eta; \lambda)}}{M^2} \left[ 1 - \frac{r_d \lambda}{2\pi M} \nabla^2 \phi(\xi, \eta; \lambda) \right]$$

(3.13)
where the absorption coefficient $\mu$ is described by

$$\mu(\xi, \eta; \lambda) = \frac{2\pi}{\lambda} \int_{\text{object}} \beta(\xi, \eta, z; \lambda) dz$$  \hspace{1cm} (3.14)$$

and $\beta$ is the complex part of the refractive index $n = 1 - \delta + i\beta$.

Since this is the theory for a generalized object, it must be applied to a specific case, which in the next section is a cylindrically shaped object.

### 3.1.2 Cylindrical phase object

Rapid variations in the boundary of an object lead to strong phase contrast as shown in the following example, even with polychromatic x-rays. Take a simple object with

![Figure 3.2: Geometry used for cross section of a cylindrical fibre](image-url)
cylindrical symmetry and refractive index, $n(k) = 1 - \delta(k)$ and negligible absorption, and surround it with a medium of refractive index $n_o = 1$, see Fig. 3.2. The phase difference for an incident plane wave through the cylindrical object with radius $r$, is

$$\phi(x, y) = 2\sqrt{r^2 - x^2 - y^2} \times (-k\delta(k)) \quad (3.15)$$

The gradient of the above (Eq. 3.15), is Eq. 3.16.

$$\nabla_{x,y}\phi = \left( \frac{-2x}{\sqrt{r^2 - x^2 - y^2}} \, \hat{i} + \frac{-2y}{\sqrt{r^2 - x^2 - y^2}} \, \hat{j} \right) (-k\delta(k)) \quad (3.16)$$

$$. \therefore \quad |\nabla_{x,y}\phi| = \frac{2\sqrt{x^2 + y^2}}{\sqrt{r^2 - x^2 - y^2}} \times (k\delta(k)) \quad (3.17)$$

The angular deviation is therefore

$$\Delta\alpha \approx \frac{1}{k} |\nabla_{x,y}\phi(x, y, z)| = 2\delta(k) \frac{\sqrt{x^2 + y^2}}{\sqrt{r^2 - x^2 - y^2}} \quad (3.18)$$

which is very large as the denominator in Eq. 3.18 $\to 0$, even though the refractive index deviation $\delta$ is very small.

Referring to Eq. 3.13, the salient points from this simple derivation are that phase contrast initially increases with increasing $r_d$ which is equivalent to defocusing [63], and that the structure of the image is proportional to the Laplacian of the projected electron density and is independent of energy to first order if $\frac{r_d\lambda}{2\pi M} \nabla^2 \phi(\xi, \eta; \lambda)$ is considered small, in which case the polychromatic spectrum can be replaced by a spectrally weighted sum and substituted for $1/k$, by neglecting the wavelength dependence of $\mu$ [65].
3.2 Wave optical approach

The basis of the wave theory was put forward by Robert Hooke (1635-1703), from observing interference phenomena in thin films and the presence of light in the geometrical shadow, as previously observed by Francesco Grimaldi (1627-1663). He proposed that light propagated instantaneously in the form of waves with rapid vibrations, and that every vibration generated a sphere in a homogenous medium. This was extended by Christian Huygens (1629-1695) with the additional assumption that every point in the aether intersected by the light wave is the source of new secondary wavelets. These spherical waves combine to form an envelope that determines the wavefront at subsequent times. Augustin Fresnel (1788-1827) gave the theory more definite form by allowing the wavelets to interfere and was able to explain diffraction from straight edges and small apertures and screens.

The basis of the scalar theory is outlined as follows. Maxwell’s equations allow a spherical wave of magnitude $E_0$ in free space emanating from the source $P_0$, located on the $z$ axis of the form,

$$E_0(r, x_0, y_0) = \frac{A e^{ikr_s}}{r_s}$$

(3.19)

where at the radial distance $r_s$, the surface has a strength $A$. This surface becomes the source of secondary wavelets propagating as spherical waves as $\frac{e^{ikr_d}}{r_d}$ to a distance $r_d$ to the observation point. The contribution from a small area $dS$ of the surface is

$$dU(P) = K(\chi) \frac{A e^{ikr_s}}{r_s} \frac{e^{ikr_d}}{r_d} dS$$

(3.20)

where $K(\chi)$ is an unknown obliquity factor that fixes the strength of the contributions.
Summing over the entire surface $S$ gives,

$$U(P) = \frac{A e^{ikr_s}}{r_s} \int \int_S K(\chi) \frac{e^{ikr_d}}{r_d} dS$$

(3.21)

Fresnel devised a unique method to evaluate the obliquity factor $K(\chi)$ based on different regions from the observation point $P$ that today are called Fresnel zones. However, Gustav Kirchhoff (1824-1887), put the ideas of Huygens and Fresnel on a sounder mathematical basis by noting that the formulation was an approximate form of a theorem by Green and Helmholtz.

### 3.2.1 Fresnel-Kirchhoff Equation

The solution to the wave equation at an arbitrary point $P$ can be expressed in terms of both the solution and its first derivative on an arbitrary closed surface surrounding $P$. If $V = U e^{-i\omega t}$ is a solution to the wave equation, then $U(P)$ is a solution to the time independent part, ie the Helmholtz equation

$$(\nabla^2 + k^2)U = 0$$

(3.22)

where $\nabla^2$ is the Laplacian operator $(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})$. Now letting $U'$ be some other function also satisfying the same requirements, then by Green’s theorem, there exists a relationship between the volume and surface integrals via

$$\int_v (U \nabla^2 U' - U' \nabla^2 U) dv = -\int_S \left( U \frac{\partial U'}{\partial n} - U' \frac{\partial U}{\partial n} \right) dS$$

(3.23)

where $\frac{\partial}{\partial n}$ is the inward normal to $S$. Following the arguments by Born and Wolf [37], this leads to the expression known as the Helmholtz-Kirchhoff formulation

$$U(P) = \frac{1}{4\pi} \int_S \left[ U \frac{\partial}{\partial n} \left( \frac{e^{ikr_d}}{r_d} \right) - \left( \frac{e^{ikr_d}}{r_d} \right) \frac{\partial U}{\partial n} \right] dS$$

(3.24)
This was extended slightly further by Kirchhoff to include polychromatic waves to

\[
V(P) = \frac{1}{4\pi} \int_S \left\{ [V] \frac{\partial}{\partial n} \left( \frac{1}{r_d} \right) - \frac{1}{r_d c} \frac{\partial V}{\partial t} - \frac{1}{r_d} \left[ \frac{\partial V}{\partial n} \right] \right\} dS \quad (3.25)
\]

Owing to mathematical complexities of these formulations Kirchhoff made certain simplifying assumptions of the boundary conditions which leads what is known as the Fresnel-Kirchhoff formulation. Using the geometry shown in Fig. 3.3, with an aperture, Kirchhoff divided the surface around \( P \) into three regions, \( A, B \) and \( C \). The contributions from regions \( B \) and \( C \) can be shown to be vanishingly small, so that only the region of the aperture may contribute. Over this area, Kirchhoff made the assumption that \( U = U^{(i)} \) and \( \frac{\partial U}{\partial n} = \frac{\partial U^{(i)}}{\partial n} \), where \( U^{(i)} \) is the incident unobstructed wave \( Ae^{i\kappa r} \). Which leads to

\[
U(P) = -\frac{Aik}{4\pi} \int \int_{\text{aperture}} \frac{e^{ik(r_s+r_d)}}{r_s r_d} [\cos(n, r_s) - \cos(n, r_d)] dS \quad (3.26)
\]

where the obliquity factor now has the explicit form of \( -\frac{ik}{4\pi} [\cos(n, r_s) - \cos(n, r_d)] \), and where \((n, r_s)\) and \((n, r_d)\) denote the angles that the radii \( r_s \) and \( r_d \) make with the screen normal \( n \).

Although this is based upon a simple aperture and spherical incident waves, the above analysis can be extended to more complicated cases. The conditional requirement is that the distances between source and observation point to the screen are large compared to the wavelength of the incident radiation, so that the radii of curvature are also large. The results are in good agreement with experiment and the Huygens-Fresnel result. Babinet’s principle also follows where the formulation of the diffraction patterns from complementary screens, \( U_1(P) \) and \( U_2(P) \), is such that

\[
U_1(P) + U_2(P) = U(P) \quad (3.27)
\]

where \( U(P) \) is the pattern formed without the screens. Use will be made of this
principle in chapter 8, for the explicit calculation of the image formed by a fibre.

Furthermore, it has been shown that Kirchhoff’s assumptions lead to an inherent inconsistency for values close to the aperture. However for most practical purposes for screens many wavelengths away from the aperture this is not a problem, and the theory turns out to be entirely adequate. Kirchhoff’s theory can be made consistent by interpreting the solution as to a somewhat different boundary condition [37] or as the average of the more self consistent Rayleigh-Sommerfeld integrals [92].

3.2.2 Rayleigh Sommerfeld Integrals

Observations that the rim of the aperture appeared to be luminous when illuminated by a light source, led Thomas Young to conjecture that the diffraction pattern observed
was the result of interference of the transmitted wave with a wave emanating from the boundary of the aperture.

Arnold Sommerfeld was able to derive a rigorous solution to the half plane diffraction problem by showing that a cylindrical wave propagated from the edge into the shadow region of the half plane, while the bright region was the interference of the original incident wave plus the cylindrical wave [37].

The question of the interference of these two waves had been investigated prior to Sommerfeld by Maggi, but was later forgotten. Rubinowicz independently investigated it and today the theory is called Maggi-Rubinowicz formulation which was developed further by Miyamoto and Wolf. For a derivation see Born and Wolf [37].

It was stated earlier that the Fresnel-Kirchhoff formulation contained some inherent inconsistency in the boundary conditions even though the application of the theory in most cases was entirely satisfactory. Due to this inconsistency other formulations are sometimes used such as the Rayleigh-Sommerfeld formulations [37]. Using a similar approximation to the Kirchhoff formulation as before, the boundary conditions become \( U \approx U^{(i)} \) on \( A \) and \( U \approx 0 \) on \( B \), but this time without the approximations of \( \frac{\partial U}{\partial z} \). The Helmholtz-Kirchhoff theory (Eq. 3.24) for observation points inside and outside the volume leads to two equations. Subtracting these from one another gives rise to the first Rayleigh diffraction integral, stated here as

\[
U(x, y, z) = \frac{1}{2\pi} \int \int_{z'=0} U(\xi, \eta, 0) \frac{\partial}{\partial z'} \left( \frac{e^{ikr_d}}{r_d} \right) d\xi d\eta \quad (3.28)
\]

where \( z' \) is a point of integration on the surface \( S \). Adding the equations gives the second Rayleigh integral

\[
U(x, y, z) = -\frac{1}{2\pi} \int \int_{z'=0} \left[ \frac{U(\xi, \eta, z')}{\partial z'} \right] \frac{e^{ikr_d}}{r_d} d\xi d\eta \quad (3.29)
\]
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When these are applied to a divergent incident wave, the boundary conditions become

\[ U^{(i)} = \frac{A e^{ik r_s}}{r_s}, \quad \frac{\partial U^{(i)}}{\partial z} = \frac{A e^{ik r_s}}{r_s} \left( ik - \frac{1}{r_s} \right) \cos(n, r_s) \]  

(3.30)

then these equations become the Rayleigh-Sommerfeld diffraction integrals

\[ U_{RS}^{(I)}(x, y, z) = \frac{1}{2\pi} \int \int_A \frac{A e^{ik r_s}}{r_s} \left( ik + \frac{1}{r_d} \right) e^{ik r_d} dS \]  

(3.31)

and

\[ U_{RS}^{(II)}(x, y, z) = -\frac{1}{2\pi} \int \int_A \frac{A e^{ik r_s}}{r_s} \left( ik - \frac{1}{r_s} \right) e^{ik r_d} dS \]  

(3.32)

Under the assumption of small angles of incidence, these equations revert to the Fresnel-Kirchhoff formula \( U_{RS}^{(I)} \approx U_{RS}^{(II)} \approx U_{FK} \). In fact the following relationship holds between the Kirchhoff and Rayleigh-Sommerfeld integrals.

\[ U^{(K)} = \frac{1}{2}(U^{(I)} + U^{(II)}) \]  

(3.33)

Although the Rayleigh-Sommerfeld integrals are more self consistent than the Fresnel-Kirchhoff theory, they are no more accurate in the vicinity of the aperture. Observation by experiment seems to support the Fresnel-Kirchhoff formulation [37]. One problem with the Rayleigh-Sommerfeld integrals is that they are restricted to apertures which the Fresnel-Kirchhoff theory is not, thereby limiting its usefulness.

3.2.3 Fraunhofer and Fresnel diffraction

Despite the accuracy of the Fresnel-Kirchhoff theory, its calculation for all but the simplest geometries is exceedingly difficult due to the highly oscillatory function in the integrand. Numerical solution requires sampling the integrand with a resolution of the order of the wavelength. Over a two dimensional aperture this requires on the order of \( N^2 \) calculations where \( N \) is number of wavelengths across an interval dimension [93].
Hence further simplifications have been sought and developed. For example, noting that though $e^{ik(r_s+r_d)}$ may vary rapidly over the area of integration, the obliquity factor $[\cos(n, r_s) - \cos(n, r_d)]$, for large distance from the aperture will change slowly and may therefore be replaced by the factor $2 \cos \zeta$, where $\zeta$ is the angle between the normal to the screen and $P_0 P$. Therefore the Fresnel-Kirchhoff equation (Eq. 3.26) becomes

$$U(P) \sim \frac{Ai \cos \zeta}{\lambda r_s r_d} \int \int_A e^{ik(r_s+r_d)} dS$$

(3.34)

where $r_s$ and $r_d$ in the denominator have been replaced by $r_s'$ and $r_d'$, which are defined with reference to schematic Fig. 3.4 as,

$$r_s'^2 = x_0^2 + y_0^2 + z_0^2$$
$$r_d'^2 = x^2 + y^2 + z^2$$

(3.35)

This can be done in a number of ways such as the method used by Born and Wolf [37], through expanding the terms $r_s$ and $r_d$ in the exponential as a Taylor series about $r_s'$ and $r_d'$ respectively.

The expansion of $r_s$ about $r_s'$ and $r_d$ about $r_d'$ in terms of the aperture plane coordinates $(\xi, \eta)$

$$r_s = r_s' - \frac{x_0 \xi + y_0 \eta}{r_s'} + \frac{\xi^2 + \eta^2}{2r_s'} - \frac{(x_0 \xi + y_0 \eta)^2}{2r_s'^3} - \ldots$$

(3.36)

Likewise for $r_d$,

$$r_d = r_d' - \frac{x_0 \xi + y_0 \eta}{r_d'} + \frac{\xi^2 + \eta^2}{2r_d'} - \frac{(x_0 \xi + y_0 \eta)^2}{2r_d'^3} - \ldots$$

(3.37)

This results in the following integral

$$U(P) = -\frac{i \cos(\delta)}{\lambda} \frac{Ae^{ik(r_s'+r_d')}}{r_s'r_d'} \int \int_A e^{ikf(\xi, \eta)} d\xi d\eta$$

(3.38)
where $\tilde{f}(\xi, \eta)$ is a function containing all the terms of the Taylor series minus $r'_s$ and $r'_d$.

$$
\tilde{f}(\xi, \eta) = -\left(\frac{x_0\xi + y_0\eta}{r'_s}\right) - \left(\frac{x\xi + y\eta}{r'_d}\right) - \frac{(x_0\xi + y_0\eta)^2}{2r'_s} - \frac{(x\xi + y\eta)^2}{2r'_s} - ... \quad (3.39)
$$
This can be further simplified by the introduction of the following variables

\[
\begin{align*}
  l_0 &= -\frac{x_0}{r'_s} \\
  m_0 &= -\frac{y_0}{r'_s} \\
  l &= -\frac{x}{r'_s} \\
  m &= -\frac{y}{r'_s}
\end{align*}
\]

(3.40)

to

\[
\tilde{f}(\xi, \eta) = (l_0-\ell)\xi-(m_0-m)\eta + \frac{1}{2} \left\{ \left( \frac{1}{r'_s} + \frac{1}{r'_d} \right) (\xi^2 + \eta^2) - \frac{(l_0\xi + m_0\eta)^2}{r'_s} - \frac{(l\xi + m\eta)^2}{r'_d} \right\} ... 
\]

(3.41)

This is important due to the two types of approximations which neglect certain orders of the \(\xi\) and \(\eta\) terms. Fraunhofer approximation neglects the higher order terms of \(\xi\) and \(\eta\) leading to an integral of the form

\[
U(P) = C \int \int_A e^{-ik(p\xi + q\eta)} d\xi d\eta
\]

(3.42)

where \(C\) is a constant containing the previous terms in front of the integral, \(p\) and \(q\) are related by

\[
p = \ell - l_0 \quad q = m - m_0
\]

(3.43)

and the condition is valid in the far field when \(r'\) and \(s'\) are sufficiently large such that

\[
|r'_s| \gg \frac{(\xi^2 + \eta^2)_{\text{max}}}{\lambda} \\
|r'_d| \gg \frac{(\xi^2 + \eta^2)_{\text{max}}}{\lambda}
\]

(3.44)

However, in the cases dealt with in this thesis, this condition is not met, therefore the Fresnel approximation is required where the quadratics in \(\xi\) and \(\eta\) must be included and higher order terms neglected.
The Fresnel approximation presents the idea of a parabolic wave approximation of the spherical wave [90]. A spherical wave emanating from a source point $P$ has the form

$$U(P) = U(r) = \frac{A}{r_s} e^{ikr_s} \tag{3.45}$$

This time, by aligning the $z$-axis with the optic axis, and considering $x$ and $y$ points not too far from the $z$-axis such that $\sqrt{x^2 + y^2} << z$ so that $\theta^2 = \frac{\sqrt{x^2+y^2}}{z} << 1$, and expanding $r_s$ as a Binomial series

$$r_s = (x^2 + y^2 + z^2)^{\frac{1}{2}} = z(1 + \theta^2)^{\frac{1}{2}} = z \left( 1 + \frac{\theta^2}{2} - \frac{\theta^4}{8} + \cdots \right)$$

$$\approx z \left( 1 + \frac{\theta^2}{2} \right) = z + \frac{x^2 + y^2}{2z} \tag{3.46}$$

Thus the spherical wave is modified to

$$U(r_s) = \frac{A}{z} e^{ikz} e^{ik\left(\frac{x^2+y^2}{2z}\right)} \tag{3.47}$$

where $r_s$ in the exponential was replaced by Eq. 3.46, while $r_s$ in the denominator is replaced by $z$ to a sufficient approximation, as it is less sensitive to errors, and thus the spherical wave has been approximated by a paraboloid.

An alternative, is to go back to the Fresnel-Kirchhoff equation Eq. 3.34, align the $z$ axis with the optic axis and have two coordinate systems, one on the aperture plane $(\xi, \eta)$ and another on the image plane $(x, y)$ see Fig. 3.5.

Rather than specify the form of the incident wave, it can be denoted arbitrarily as $U(\xi, \eta, 0)$ so that the amplitude of the field at a point $P$ is written as

$$U(x, y, z) = \frac{i}{\lambda} \int \int_A U(\xi, \eta, 0) \frac{e^{ikr_d}}{r_d} \cos \zeta \ d\xi d\eta \tag{3.48}$$
The Fresnel approximation makes this

\[ U(x, y, z) = \frac{i}{\lambda} \frac{e^{ikz}}{z} \int \int_A U(\xi, \eta, 0) e^{\frac{ik}{z}[(x-\xi)^2 + (y-\eta)^2]} d\xi d\eta \] (3.49)

with the usual paraxial approximation \( \cos \zeta = 1 \). This equation is important due to its separability as long as the transmission function \( U(\xi, \eta, 0) \) can be written as \( U(\xi, \eta, 0) = U_x(\xi)U_y(\eta) \). If higher terms in the expansion had been kept, the cross terms would not enable this separability [94]. As noted by Fieock [95], Eq. 3.49 is an exact solution of the paraxial equation

\[ \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} - 2ik \frac{\partial}{\partial z} \right) U = 0 \] (3.50)

as long as the factor \( e^{ikz} \) is left out.

For numerical computation purposes, the two dimensional integral can be simplified by Cowley’s method [96] to a one dimensional integral by assuming that \( U(\xi, \eta) \) only

Figure 3.5: Aperture plane and image plane with \( z \) aligned along optic axis
varies in the $\xi$ direction, so that the $\eta$ integral can be taken out and performed separately

$$\int_{-\infty}^{\infty} e^{-ik(y-\eta)^2/2z} d\eta = \sqrt{\frac{z\lambda}{i}}$$  (3.51)

Furthermore, limiting the aperture in the $\xi$ direction to a width $2a$, the integral becomes

$$U(x, z) = \sqrt{\left(\frac{i}{z\lambda}\right)} e^{-ikz} \int_{-a}^{a} U(\xi, 0) e^{-ik(x-\xi)^2/2z} d\xi$$  (3.52)

In comparisons with computational analysis compared to an exact Rayleigh-Sommerfeld (I) formulation, the Fresnel approximation shows almost no errors for an incident plane wave, for an aperture in the far and extreme near field even for high Fresnel numbers. For an incident spherical wave the errors are predominately phase errors [94].

### 3.3 Fourier Optics

A different approach to solving the diffraction integral is the linear systems theory approach of treating the optical disturbance of an object in the beam as a linear superposition of plane waves and applying a transfer function [97]. In this approach, the diffraction problem is split into two parts: one in which the effect of the obstacle or screen has on the field immediately afterwards, and two, the propagation of the effect further downstream of the obstacle, i.e. the extent of the effect. Thus an optical system can be described in terms of a linear systems theory as an input which is modified by the system and mapped to an output. The system is then characterized by either an impulse-response, which is the response to a point input, or transfer function which is the response to spatial harmonic functions [90].

An arbitrary wave in free space can be analyzed as a superposition of plane waves, and the transmission through lenses, apertures and free space can be viewed in terms of Fourier transforms of these components. By analogy with the dispersion of frequencies in a prism, free space propagation can serve as a spatial prism.
Since, in this thesis Fresnel diffraction is used extensively, only the theory relevant to the Fourier representation of Eq. 3.49 will be presented. This can be obtained by converting $k$ into $k = \frac{2\pi}{\lambda}$ and expanding the squares of the exponential in the integral.

\[(x - \xi)^2 = x^2 + \xi^2 - 2x\xi\]

\[(y - \eta)^2 = y^2 + \eta^2 - 2y\eta\]  

so that Eq. 3.49 becomes

\[U(x, y, z) = i\frac{\lambda}{z} e^{ikz} \iint_{\text{aperture}} U(\xi, \eta, 0) e^{\frac{i\pi}{\lambda z}(-2x\xi + \xi^2 - 2y\eta + \eta^2)} d\xi d\eta \] (3.54)

Rearranging this slightly

\[U(x, y, z) = i\frac{e^{ikz}}{\lambda z} e^{\frac{i\pi}{\lambda z} (x^2 + y^2)} \int \int_{-\infty}^{\infty} \left[U(\xi, \eta, 0)e^{\frac{i\pi}{\lambda z} (\xi^2 + \eta^2)}\right] e^{\frac{i\pi}{\lambda z}(-2x\xi - 2y\eta)} d\xi d\eta \] (3.55)

where the limits have been extended to $+\infty$ to $-\infty$, and the aperture has been incorporated into $U(\xi, \eta, 0)$. Now the integral is the Fourier transform of the aperture function and a quadratic phase factor. Defining the Fourier transform of an arbitrary function $g(x, y)$ as

\[G(p, q) = \mathcal{F}[g(x, y)] \equiv \int \int_{-\infty}^{\infty} g(x, y) e^{-2\pi i (px + qy)} dx dy \] (3.56)

where capital letters of a function denote its Fourier transform, then the Fresnel integral may now be written as

\[U(x, y, z) = i\frac{e^{ikz}}{\lambda z} e^{\frac{i\pi}{\lambda z} (x^2 + y^2)} \mathcal{F} \left[U(\xi, \eta, 0)e^{\frac{i\pi}{\lambda z} (\xi^2 + \eta^2)} \right] \bigg|_{p = \frac{x}{\lambda z}, q = \frac{y}{\lambda z}} \] (3.57)

This is an equivalent form of the Fresnel diffraction integral of Eq. 3.49. Another important relation is that this integral can also be written as a convolution integral.
Repeating Eq. 3.49,

\[ U(x, y, z) = \frac{i}{\lambda} e^{ikz} \int \int U(\xi, \eta, 0) e^{\frac{ik}{z} [(x-\xi)^2 + (y-\eta)^2]} d\xi d\eta \] (3.58)

it may be seen that the convolution integral is the same

\[ U(x, y, z) = \int \int U(\xi, \eta, 0) h(x - \xi, y - \eta) d\xi d\eta \] (3.59)

where the function \( h(x, y) \) is

\[ h(x, y) = \frac{i}{\lambda} e^{\frac{i\pi}{\lambda z} (x^2 + y^2)} \] (3.60)

Hence

\[ U(x, y, z) = \frac{e^{ikz}}{z} U(x, y, 0) \ast h(x, y) \] (3.61)

where \( \ast \) denotes two dimensional convolution. The Fourier transform of \( h(x, y) \) is \( H(p, q) \) and is called the transfer function of free space. These forms will be used extensively in chapter 8, where an explicit derivation is given for the simulations performed in this thesis.

### 3.3.1 Angular spectrum

An arbitrary monochromatic wave incident upon an aperture may be expressed as the sum of monochromatic plane waves through the inverse Fourier transform

\[ U(x, y, z = 0) = \int \int_{-\infty}^{\infty} \hat{U}(f_X, f_Y; 0) e^{2\pi i (fx + fy y)} df_X df_Y \] (3.62)

A plane wave with a component in the \( z \) direction may be written as

\[ e^{ik \cdot r} = e^{i(k_x x + k_y y + k_z z)} \] (3.63)
the magnitude of the wave vector $k$ is $|k| = \frac{2\pi}{\lambda}$, therefore the directions of $k$ may be written in terms of direction cosines $(\alpha, \beta, \gamma)$, where the condition $\gamma = \sqrt{1 - \alpha^2 - \beta^2}$ must be satisfied. The plane wave is now

$$e^{ikr} = e^{\frac{2\pi i}{\lambda}(ax + \beta y + \gamma z)} = e^{\frac{2\pi i}{\lambda}(ax + \beta y)} e^{\frac{2\pi i}{\lambda}\gamma z}$$  \hspace{1cm} (3.64)$$

At the plane $z = 0$, this reduces to $e^{\frac{2\pi i}{\lambda}(ax + \beta y)}$ which must be equated with the inverse Fourier transform exponential $e^{2\pi i(f_x x + f_y y)}$, with $\alpha = f_x \lambda$, $\beta = f_y \lambda$ and $\gamma = \sqrt{1 - (f_x \lambda)^2 - (f_y \lambda)^2}$. The inverse Fourier transform also expresses the decomposition of $U(x, y; 0)$ as a sum of plane waves with weighting factors $\hat{U}(f_x, f_y; 0)$, evaluated at frequencies $f_x = \alpha/\lambda$ and $f_y = \beta/\lambda$. These weighting factors are the angular spectrum of the disturbance at $U(x, y, z = 0)$.

$$A_s(\frac{\alpha}{\lambda}; \frac{\beta}{\lambda}; 0) = \int \int_{-\infty}^{\infty} U(x, y; 0) e^{-2\pi i(\frac{\alpha}{\lambda} x + \frac{\beta}{\lambda} y)} dx dy$$ \hspace{1cm} (3.65)$$

The conditions for the rigorous validity of these derivations have been investigated by Lalor [98], for the necessary and sufficient conditions of the integrals of the wavefield $U(x, y; z)$. He also shows how an exact solution of the Helmholtz equation is given by the second Rayleigh-Sommerfeld integral.

$$U(x, y; z) = -\frac{1}{2\pi} \int \int_{-\infty}^{\infty} U(\xi, \eta; 0) \frac{\partial}{\partial z} \left( \frac{e^{ikr_d}}{r_d} \right) d\xi d\eta$$ \hspace{1cm} (3.66)$$

### 3.3.2 Propagation of Angular Spectrum

The effect of propagation of the angular spectrum is determined by calculating $A_s(\frac{\alpha}{\lambda}, \frac{\beta}{\lambda}, z)$

$$A_s(\frac{\alpha}{\lambda}, \frac{\beta}{\lambda}; z) = \int \int_{-\infty}^{\infty} U(x, y, z) e^{-2\pi i(\frac{\alpha}{\lambda} x + \frac{\beta}{\lambda} y)} dx dy$$ \hspace{1cm} (3.67)$$

where the relationship between $A_s(\frac{\alpha}{\lambda}, \frac{\beta}{\lambda}; z)$ and $A_s(\frac{\alpha}{\lambda}, \frac{\beta}{\lambda}; 0)$ is determined by the Helmholtz equation $\nabla^2 U + k^2 U = 0$. Performing the inverse Fourier transform
on Eq. 3.67 and substituting into Helmholtz’s equation results in the solution (see Goodman [99])

\[
A_s(\frac{\alpha}{\lambda}, \frac{\beta}{\lambda}; z) = A_s(\frac{\alpha}{\lambda}, \frac{\beta}{\lambda}; 0)e^{\frac{2\pi iz}{\lambda}\sqrt{1-\alpha^2-\beta^2}}
\]  

(3.68)

when \(\alpha^2 + \beta^2 < 1\) corresponding to propagating waves and

\[
A_s(\frac{\alpha}{\lambda}, \frac{\beta}{\lambda}; z) = A_s(\frac{\alpha}{\lambda}, \frac{\beta}{\lambda}; 0)e^{-\frac{2\pi iz}{\lambda}\sqrt{\alpha^2+\beta^2-1}}
\]  

(3.69)

when \(\alpha^2 + \beta^2 > 1\), which corresponds to evanescent waves. These conditions restrict the range of frequencies when inverse transforming Eq. 3.67

\[
U(x, y; 0) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} A_s(\frac{\alpha}{\lambda}, \frac{\beta}{\lambda}; 0)e^{\frac{2\pi iz}{\lambda}\sqrt{1-\alpha^2-\beta^2}}
\times \text{circ}(\sqrt{\alpha^2 + \beta^2})e^{2\pi i(\frac{\alpha}{\lambda}x + \frac{\beta}{\lambda}y)}d\frac{\alpha}{\lambda}d\frac{\beta}{\lambda}
\]  

(3.70)

Now the solution to Helmholtz’s equation for propagating waves in terms of frequencies can be written with the inclusion of the \text{circ} function to

\[
A_s(f_X, f_Y; z) = A_s(f_X, f_Y; 0)\text{circ}(\sqrt{(\lambda f_X)^2 + (\lambda f_Y)^2})e^{\frac{2\pi iz}{\lambda}\sqrt{1-(\lambda f_X)^2-(\lambda f_Y)^2}}
\]  

(3.71)

This leads to an expression for the transfer function \(H(f_X, f_Y) = \mathcal{F}[h(x, y)]\)

\[
H(f_X, f_Y) = \begin{cases} 
  e^{\frac{2\pi iz}{\lambda}\sqrt{1-(\lambda f_X)^2-(\lambda f_Y)^2}}, & \text{where } \sqrt{f_X^2 + f_Y^2} < \frac{1}{\lambda} \\
  0, & \text{otherwise}
\end{cases}
\]  

(3.72)

which is also valid outside the near field.

### 3.3.3 Fresnel Approximation and Angular Spectrum

There remains to establish a link with the Fresnel approximation and the angular spectrum. It was stated before that the transfer function \(H(f_X, f_Y)\) in the Fresnel
approximation is just the Fourier transform of the impulse response \( h(x, y) \). Specifically

\[
H(f_X, f_Y) = F\left[ h(x, y) = \frac{e^{j\lambda z}}{j\lambda} e^{i\pi(x^2+y^2)} \right] = e^{ikz} e^{-i\pi\lambda z} (f_X^2 + f_Y^2)
\]

The relationship shows that the quadratic spatial dispersion becomes a quadratic frequency dispersion of the plane waves travelling in different directions with a constant phase factor \( e^{ikz} \) in front. Comparing this with the more general equation derived previously Eq. 3.72, the phase term \( \sqrt{1 - (\lambda f_X)^2 - (\lambda f_Y)^2} \) may be approximated by the Binomial theorem to

\[
\sqrt{1 - (\lambda f_X)^2 - (\lambda f_Y)^2} \approx 1 - \left[ \frac{(\lambda f_X)^2 + (\lambda f_Y)^2}{2} \right]
\]

which is only valid if the terms \( (\lambda f_X)^2 \ll 1 \) and \( (\lambda f_Y)^2 \ll 1 \), which simply restricts \( f_X \) and \( f_Y \) to small angles. Hence the connection with the angular spectrum is equivalent to the paraxial approximation.

Greater detail of the various derivations of Fresnel equation and their comparisons are given by Southwell [94].

### 3.4 Transmission function

So far only apertures have been considered and a modification is needed to handle objects which alter the phase and amplitude of an incident wave. Thus the equation is modified for a partially transmitting aperture or object by use of a transmission function \( q(\xi, \eta) \) [96]. In what follows, most transmission functions are those of phase objects. An everyday example is the thermal density fluctuations in air [100]. Generally though, a phase object is considered to have some absorption or some multiple scattering so that there is a mixture of phase and amplitude contrast. However, there exists a large class of objects especially biological objects whose transmission
function can be considered as pure phase objects as a reasonable approximation, where it is understood that the object is thin enough so that phase contrast dominates the amplitude contrast \[96\]. In most papers reviewed, the object of consideration is assumed to have weak absorption and to vary only appreciably in one direction say the $\xi$-direction. This is to greatly simplify calculation, as two dimensional integrations are numerically expensive and hence the transmission function is usually written as

$$q(\xi) = e^{i\phi(\xi) - \mu(\xi)} \quad (3.75)$$

where $\phi$ is the phase and $\mu$ is the absorption. The transmission function is related to the real $\delta$ and imaginary $\beta$ parts of the refractive index $n = 1 - \delta + i\beta$, through the following relations

$$\mu(x, y) = \frac{2\pi}{\lambda} \int \beta(x, y, z) dz \quad (3.76)$$
$$\phi(x, y) = \frac{2\pi}{\lambda} \int [1 - \delta(x, y, z)] dz = \phi_0 - \frac{2\pi}{\lambda} \int \delta(x, y, z) dz \quad (3.77)$$

with $\phi_0$ a constant phase term. The object’s intensity transmission function is $|q(\xi)|^2 = e^{-2\mu(\xi)}$.

### 3.4.1 Phase edge

The simplest type of phase object is a phase step with an abrupt change of phase near the edge \[60\]. For a plane wave as shown in Fig. 3.6, a relationship may be readily derived for $q(\xi)$. In this case the plane wave has the form $e^{ikz}$, and passing through the object causes a phase shift proportional to the thickness $\tau$. This may be also be considered as the wavenumber $k$ changing by the refractive index of the material to $k_n = \frac{2\pi}{\lambda_n} = \frac{2\pi}{\lambda \cdot n} = \frac{2\pi n}{\lambda} = kn$. Thus by making the simplification that the phase change
is constant over the thickness of the material, the difference at the boundary is

\[ iknt - ikt = ik(n - 1)\tau \]
\[ = ik(-\delta + i\beta)\tau \]
\[ = -i k\delta\tau - k\beta\tau \]

Hence the transmission function \( q(\xi) \) for an edge located on \( \xi = 0 \), may be written in the form

\[ q(\xi) = \begin{cases} 1 & \text{if } \xi \geq 0, \\ e^{-i k\delta\tau - k\beta\tau} & \text{if } \xi < 0. \end{cases} \]

A derivation along these lines was performed by Margaritondo and Tromba \[101\] for an edge located at position \( \xi_0 \), which they called a variation of the classical opaque edge treatment. With the modification that the edge is partially transmitting the amplitude of the wavefield \( U \) is modified to

\[ U(x, y) \propto [C(\infty) - C(-u_0)] + i[S(\infty) - S(-u_0)] \\
+ e^{-\mu + i\phi}[C(\infty) - C(-u_0)] + i[S(\infty) - S(-u_0)] \]

where \( \mu \) is the attenuation coefficient and \( \phi \) is the phase shift, and \( u_0 = u(\xi_0) \) is a reduced variable \( u(z) = z\sqrt{2(r_s + r_d)/r_s r_d \lambda} \). Again under the assumption of small \( \mu \)
and $\phi$, the intensity is approximately

$$I(x, y) \propto 1 - \mu + \phi [C(-u_0) - S(-u_0)] - \mu [C(-u_0) - S(-u_0)]$$ (3.81)

A further approximation for $\mu < \phi$ reduces this equation to

$$I(x, y) \propto 1 + \phi [C(-u_0) - S(-u_0)] - \mu [C(-u_0) - S(-u_0)]$$ (3.82)

From this the Cornu spiral is used to give a maximum intensity $I$ at $u_0 = 0.7$, which they claim is the main form of image sharpening. Simulated images are compared to experimental ones in Fig. 3.7, however they point out that comparison is made difficult since real objects are complex and depart from ideal straight edges. Originally straight edges were used in this thesis, but the difficulty in obtaining a straight enough edge soon became apparent, and hence better phase contrast images were obtained with fibres.

### 3.4.2 Cylindrically shaped phase objects

For a cylindrically shaped object such as a uniform fibre, with the long dimension oriented along the $\eta$ axis such as shown in Fig. 3.8, the transmission function as per Monnin [42] in the case of plane waves is

$$q(\xi, \eta) = e^{-\frac{4\pi}{\lambda} (\theta+i\delta) \sqrt{r_0^2 - \xi^2}}$$ (3.83)

A detailed mathematical derivation for a cylindrical hollow fibre will be presented in chapter 8 for the refraction simulations. Other examples of phase objects with simple symmetry are: cylindrical holes drilled in 1 mm thick plastic, by Hong et al [102], Latex spheres by Mayo et al [103], voids of air in adhesive by Stevenson et al [104], and human tooth dentin as used by Zabler et al [105].
Figure 3.7: Top: simulated image of strip shaped object, with standard absorption image on left compared to coherence-enhanced image right. Bottom: experimental image enhancement from Margaritondo and Tromba [101]


\[ U(x, y) = U_0(x, y)[1 + c(x, y)] \] (3.84)

where the function \( c(x, y) \) contains the diffraction integral in a slightly modified form, in that the phase function \( e^{i\phi(\xi, \eta)} \) in the object plane is replaced by \( e^{i\phi(\xi, \eta)} - 1 \)

\[
c(x, y) = \frac{M}{i\lambda s} e^{i\pi \left[ \frac{(x-x_0)^2}{(r+s)} + \frac{(y-y_0)^2}{(r+s)} \right]} \\
\times \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} d\xi d\eta (e^{i\phi(\xi, \eta)} - 1) e^{i\pi \left[ \frac{(\xi-x_0)^2}{2} + \frac{(\eta-y_0)^2}{2} + \frac{\xi^2}{2s} + \frac{\eta^2}{2s} \right]} (3.85)
\]
The transmission phase function \( \phi(\xi, \eta) \) is broadened to include attenuation to \( \Phi(\xi, \eta) = \phi(\xi, \eta) + \mu(\xi, \eta) \), where

\[
\phi(\xi, \eta : \lambda) = -\frac{2\pi}{\lambda} \int_{\text{object}} \delta(\xi, \eta, z : \lambda) dz
\]

and

\[
\mu(\xi, \eta : \lambda) = \frac{2\pi}{\lambda} \int_{\text{object}} \beta(\xi, \eta, z : \lambda) dz
\]

The intensity, normalized is calculated to be

\[
I(x, y) = 1 + c(x, y) + c^*(x, y) + |c(x, y)|^2
\]

(3.86)

With a Fourier transform this becomes

\[
\hat{I}(u, v) = \delta(u, v) + C(u, v) + C^*(-u, -v) + A(u, v)
\]

(3.87)

where \( C(u, v) \) the Fourier transform of \( c(x, y) \) is defined by

\[
C(u, v) = M^2 \Phi(Mu, Mv) e^{-\pi \lambda s M (u^2 + v^2)} e^{i2\pi (\frac{sx_0}{r}) u + 2\pi (\frac{sy_0}{r}) v} \]

(3.88)

The term \( e^{-\pi \lambda s M (u^2 + v^2)} \) represents the optical transfer function (OTF) for Fresnel diffraction, and in frequency space behaves like a filter. The term \( \Phi(Mu, Mv) \) is the Fourier Transform of \( e^{i\Phi(\xi, \eta)} - 1 \), scaled by the magnification factor \( M \). Thus Eq. 3.88 and 3.85 represent alternative methods of calculating phase contrast signals, with the notable difference that Eq. 3.85 must be calculated via numerical integration.

The remaining term \( A(u, v) \) which is the Fourier transform of \( |c(x, y)|^2 \) is described
by the invocation of the Wiener-Khincin (or Wiener-Khinchin [106]) theorem to be

\[
A(u, v) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} d\alpha d\beta \ C^*(\alpha, \beta) C(\alpha + u, \beta + v) \\
= e^{2\pi \left(\frac{\alpha u}{\lambda r} + 2\pi \frac{\beta v}{\lambda r}\right)} \\
\times \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} d\alpha d\beta \ M^4 \Phi^*(M\alpha, M\beta) \Phi[M(\alpha + u), M(\beta + v)] e^{-2\pi i \lambda r M(\alpha u + \beta v)}
\]

however this term is often neglected in the weak object condition since it is of second order. The effect of the source and detector are modelled by convolution

\[
I_{\text{conv}} = [I(x, y) * \text{PSF}_{\text{geom}}(x, y)] * \text{PSF}_{\text{det}}(x, y)
\]

where * represents convolution, and \(I_{\text{conv}}\) represents the x-ray intensity signal \(I(x, y)\) convolved with the point spread function (PSF) of the source and detector. This has the effect of smearing the image somewhat and will be used in this thesis explicitly in chapter 8.

A commonly used assumption for the x-ray microsource is a circular source [107] or Gaussian [108], [109]. For image plate detectors the PSF can be approximated as a Lorentzian as stated by Cookson [110] when used with a monochromatic synchrotron source (\(\lambda = 1.2\AA \approx 10\ \text{keV}\)) or Lorentzian/Gaussian as shown by Seely et al [111] using a tungsten based laboratory source, depending on the thickness of phosphor and binder used in the image plate. Cookson found the full width, half maximum (FWHM) value for the Lorentzian to be 0.126 mm for a 10 keV beam using a BAS2000 scanner and an unspecified Fuji image plate. Seely et al found the FWHM the width of the PSF was found to be 0.13 mm FWHM Gaussian for Fuji Superior Resolution (SR) to 0.19 mm FWHM Lorentzian which includes the scanner contribution for Fuji Maximum Sensitivity (MS) when a narrow 11.268 keV (W L\(_\gamma\)) spectral line was used see Fig. 3.10. Energy dependence of the FWHM value was found to vary by Bourgeois et al [112] from 0.142 mm for 10 keV to 0.130 mm for 40 keV, also using a BAS2000
CHAPTER 3. PHASE CONTRAST THEORY

Figure 3.9: Focal spot image and corresponding line profile of the Nova600 (Oxford Instruments) x-ray microfocus source showing a Gaussian type distribution [108]

Figure 3.10: (a) MTF of the SR and MS image plates. (b) The corresponding point spread functions where curve 1 is for the SR image plate, 2 is for the MR plate, 3 is the SR image plate PSF convolved with the scanner PSF, and 4 is the MS PSF convolved with the scanner PSF [111]

scanner and unspecified image plate.
3.4.4 Summary

This chapter has outlined the theory of phase contrast image formation from the convenience and simplicity of geometric optics to the more accurate and complex wave diffraction theory. Analysis from geometrical optics reveals that although the phase shift through an object such as a fibre may be very slight, it can lead to large refraction angles (Eq. 3.18) resulting in measurable intensity changes at the detector plane (Eq. 3.13). The scalar wave approach is based on the Helmholtz equation which in turn is based on Maxwell’s equations, and after application of Green’s theorem, leads to propagation models such as the Fresnel-Kirchhoff and Rayleigh-Sommerfeld integrals. The different diffraction patterns produced by these are due to different aspects of the boundary conditions. However, despite their accuracy, these formulations are difficult to implement except for very simple geometries and therefore various approximations such as Fresnel and Fraunhofer methods are used in practice.

The Fourier optical approach, which is equivalent to the wave optical approach, is also outlined since it will be used extensively in Chapter 8. The wavefield at the detector is a convolution of the wavefield at the object plane and the impulse response of the system. The disturbance of the wavefield at the detector can be decomposed into a sum of plane waves, with weighting factors that are the angular spectrum. The propagation of the angular spectrum produces conditions that result in propagated waves and evanescent waves, which leads to an expression of the transfer function of free space. Using the Binominal theorem approximation on the transfer function effectively restricts the angles which leads to a connection of the Fresnel approximation as being equivalent to the paraxial approximation.

A brief mention for completeness is made of a third approach based on Wigner distributions (Wu and Lui [113], [114], Donnelly et al [115], Chapman [80]) which takes into account the spatial coherence of the source and hence is more general than the Fresnel-Kirchhoff method [91]. However, in this thesis, the micro-focus source has been modelled as incoherent and therefore this approach has not been used.
The wave and geometric ray formulations are equivalent when the source and detector convolutions are taken into account. The object transmission function has been determined for both the weak and moderate phase condition for the simple cases of an edge and a fibre. In the case of a phase edge, the Fresnel-Kirchhoff equation can evaluated using Fresnel Sine and Cosine integrals. It remains now to simulate the refraction and diffraction cases computationally and compare them to experiment.
Chapter 4

Interaction of x-rays with matter

The process of diffraction as described in the previous chapter can be viewed as a convolution of two separate and simultaneous operations, namely scattering and interference [116]. This chapter broadens the image formation process and places it within the general framework of scattering. Scattering of electromagnetic radiation is one of the fundamental ways of probing the internal structure and dynamics of matter. When the primary radiation is tuned so that the index of refraction of the material is close to unity, the scattered radiation results mainly from primary interactions between the radiation and the electrons in the medium, which can be considered free in the first approximation [117]. Previously, the complex index of refraction, \( n = 1 - \delta + i\beta \), was used to characterize the way x-rays interacted with matter but little was said about how the values for \( \delta \) and \( \beta \) were obtained. Examination of this aspect leads to the interaction between x-rays and matter and scattering theory. For the tube potentials in the range of 30-150kVp, as used in this thesis, there are three interactions of particular interest: photoelectric absorption, coherent and incoherent scattering. A short review of these will be presented before the author’s own model of incoherent scatter is used to calculate the effect on phase contrast from the object and the introduction of filters.
4.1 Attenuation, absorption and extinction

Absorption, attenuation and extinction are terms used often used interchangeably to describe the reduction as x-rays as they traverse matter [90], [37]. Extinction was a term introduced by Darwin (1914) to explain observed differences in crystallography from the kinematical approximation [96]. It is also used in astronomy to describe the absorption and scattering of electromagnetic radiation by matter such as dust and gas between an emitting object and the observer [118]. In infrared optics, the extinction coefficient $\kappa$ is part of the complex refractive index $\hat{n} = n - i\kappa$, while the absorption coefficient is related to it by $\alpha = \frac{2\kappa}{\omega}$, where $\omega$ is the angular frequency and $c$ is the speed of light [119]. For visible light, the attenuation $\mu$ as an approximation [120], is the sum of absorption $\chi$ and scattering $s$,

$$\mu = \chi + s \quad (4.1)$$

In diffraction enhanced imaging (DEI), Oltulu et al describe a process of separating absorption and extinction in relation to the monochromator rocking curve [121]. For the purposes of this thesis though, attenuation and extinction will be treated as the same so that when an x-ray beam passes through matter, it undergoes attenuation via the processes of scattering and absorption (see Fig. 4.1). Quantitatively it can be described by the linear attenuation coefficient $\mu$ or $\alpha_e$ and the Bouger-Lambert-Beer law

$$I(x) = I_0e^{-\mu x} \quad (4.2)$$

where $I(x)$ is the intensity of the beam at a distance $x$ through a material object and $I_0$ is the incident intensity. The above definition is applicable under conditions of monochromaticity, narrow beam geometry and a homogeneous target material [122]. When an inhomogeneous object is irradiated by a polychromatic beam, as is the case for radiography and computed tomography, it is modified by energy dependent factors.
where \( r = (\alpha, d) \) is the vector representation of the line traversed \( l_{\alpha,d} = \{x : \alpha \cdot x = d\} \) and \( \alpha \) is a direction vector, \( d \) is the direction from the origin, and \( S(E) \) is the beam spectrum profile [123]. The linear attenuation coefficient is related to the cross section \( \sigma \) and atomic density \( \rho_a \) by [124]

\[
\mu = \rho_a \sigma
\]  

(4.4)

and also related to the mass attenuation coefficient \( \mu_m \) by [125]

\[
\mu_m = \frac{\mu}{\rho}
\]

(4.5)

An example of the various components of the mass attenuation coefficient for water from calculations of the XCOM [127] program is shown in Fig. 4.2. Tabulated values of \( \frac{\mu}{\rho} \) such as Hubbell [128] rely on theoretical values for the total cross section per atom,
Figure 4.2: Attenuation coefficients calculated from the XCOM program for water [126]

\[ \sigma_{tot}, \text{ which is related to } \frac{\mu}{\rho} \text{ according to } \]

\[ \frac{\mu}{\rho} = \frac{\sigma_{tot}}{uA} \] \hspace{1cm} (4.6)

where \( u = 1.6605402 \times 10^{-24}\text{g} \) is the atomic mass unit, which is defined as \( \frac{1}{12} \) of the mass of a \(^{12}\text{C}\), \( A \) is the relative atomic mass of the target element, and \( \sigma_{tot} \) is the total cross section in barns/atom, where \( \text{barn} = 10^{-24} \text{ cm}^2 \) [129]. The attenuation coefficient and cross sections are functions of x-ray energy, and the total cross section over a broad
energy range can be written as a sum of contributions as

$$\sigma_{\text{tot}} = \sigma_{\text{pe}} + \sigma_{\text{coh}} + \sigma_{\text{incoh}} + \sigma_{\text{pair}} + \sigma_{\text{trip}} + \sigma_{\text{ph.n}}$$  \hspace{1cm} (4.7)

where $\sigma_{\text{pe}}$, is the photoelectric cross section, $\sigma_{\text{coh}}$ is the coherent or Rayleigh cross section, $\sigma_{\text{incoh}}$ is the incoherent or Compton cross section, $\sigma_{\text{pair}}$ and $\sigma_{\text{trip}}$ are the electron-positron cross sections produced in the nuclear field by pair production ($1e^-, 1e^+$) and atomic electron field by triplet production ($2e^-, 1e^+$) respectively and $\sigma_{\text{ph.n}}$ is the photonuclear cross section. Fig. 4.3 shows the relative amounts of the different cross sections for carbon over a large energy range, where the photoelectric cross section $\sigma_{\text{pe}}$ is denoted by $\tau$. For the energies considered in this thesis ($\leq 10^6 eV$), it can be seen that only $\sigma_{\text{pe}}$, $\sigma_{\text{coh}}$ and $\sigma_{\text{incoh}}$ are significant.

4.1.1 Absorption

Absorption is defined as the progressive conversion of the incident beam into different forms of energy and matter such as heat by absorption, inelastic scatter and electron-positron pair production. Elastic scattering is not included as it re-emits the radiation without change of energy [131]. The photoelectric effect or photoeffect is the main absorber of x-ray photons below 30 keV. Dramatic examples of some medical absorption images are shown in Fig. 4.4, where it does not take much expertise to diagnose the causes of these headaches!

In the quantum picture, an x-ray photon may be photoelectrically absorbed by an atom if the energy of the photon is sufficient to eject an inner core electron from an atom as depicted in Fig. 4.5. The cross section varies approximately as $Z^4$, where $Z$ is the atomic number of the material and can be followed by the processes of fluorescence and Auger emission [124]. For the energies and light element materials considered here though, fluorescence is so low in energy and intensity, that for practical purposes it is negligible [133].
Thus incoherent scattering and the photoelectric effect are predominantly responsible for absorption contrast in practical radiography at diagnostic energies. Where x-ray dose is concerned, there is a trade-off between maximizing this effect for good contrast while limiting the dose from ionization. Therefore filters, typically aluminium and copper are used to enhance the photoeffect by absorbing lower energies that contribute little to diagnostic information but add considerably to patient dose. Kerma is the term used in reference to dose which is an acronym for the sum of the kinetic energies of primary charged particles released by the incident photons per unit mass [125].
Chapter 4. Interaction of X-rays with Matter

(a) Knife attack  (b) Archery accident

Figure 4.4: Some extreme examples of medical absorption images (Both survived!) [132]

Figure 4.5: Photoelectric absorption of an x-ray by an atom

The attenuation of x-rays by different tissue types in the body is determined by their elemental and chemical compositions. The three tissue types of interest are: adipose tissue (fat), striated tissue (soft), and bone [134]. They are tabulated in Table 4.1 together with their elemental compositions. Since soft tissue includes muscle and body fluids, which are about 75% and 85-100% water by weight respectively, they are often treated as equivalent to water with an effective atomic number of 7.4 and an electron density of $3.34 \times 10^{26}$ electrons per gram [134]. Referring to Fig. 4.6, it can be observed that the photoelectric effect dominates photon attenuation in water to 30 keV, after which the Compton effect becomes increasingly dominant. However, it is the photoelectric interactions that provide better differentiation between the various tissue types and why it is desirable to use lower energy photons in diagnostic examinations.
CHAPTER 4. INTERACTION OF X-RAYS WITH MATTER

Table 4.1: Composition of body tissues from Lancaster [134]

<table>
<thead>
<tr>
<th>Composition (by mass)</th>
<th>Adipose Tissue (fat)</th>
<th>Muscle (striated) (soft tissue)</th>
<th>Water</th>
<th>Bone (Femur)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen (Low Z)</td>
<td>11.2</td>
<td>10.2</td>
<td>11.2</td>
<td>8.4</td>
</tr>
<tr>
<td>Carbon</td>
<td>57.3</td>
<td>12.3</td>
<td></td>
<td>27.6</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>1.1</td>
<td>3.5</td>
<td></td>
<td>2.7</td>
</tr>
<tr>
<td>Oxygen</td>
<td>30.3</td>
<td>72.9</td>
<td>88.8</td>
<td>41.0</td>
</tr>
<tr>
<td>Sodium</td>
<td></td>
<td>0.08</td>
<td></td>
<td>0.2</td>
</tr>
<tr>
<td>Magnesium</td>
<td></td>
<td>0.02</td>
<td></td>
<td>0.2</td>
</tr>
<tr>
<td>Phosphorus</td>
<td></td>
<td>0.2</td>
<td></td>
<td>7.0</td>
</tr>
<tr>
<td>Sulfur</td>
<td>0.06</td>
<td>0.5</td>
<td></td>
<td>0.2</td>
</tr>
<tr>
<td>Potassium</td>
<td></td>
<td>0.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Calcium (High Z)</td>
<td></td>
<td>0.007</td>
<td></td>
<td>14.7</td>
</tr>
</tbody>
</table>

Contrast for these tissues is dictated predominantly by variations in the thickness or density so that thickness differences of about 3 cm produce a radiologic contrast of about 50%. Unfortunately, the radiographic similarity of a majority of tissue volume in the human body complicates the imaging task. For example, visualizing the blood vessels directly or to separate tumors from surrounding normal soft tissue is nearly impossible without the use of iodine contrast agents. This improves the radiographic contrast of anatomical structures of interest such as the liver, gastrointestinal tract, and cardiac blood pool, via standard plane film techniques [134]. This is an area of potential improvement offered by phase contrast imaging since the phase coefficient is far greater than the absorption coefficient, eliminating the need of a chemical contrast agent.

4.2 Scattering

The alternative to absorption of x-rays in its interaction with matter, is scattering which occurs in two forms. Historically these two forms were observed in 1896 by Imbert and Bertin-Sans in x-ray reflectivity experiments. They concluded that x-rays were
scattered rather than reflected from common objects. Furthermore, the scattered beam consisted of two components. An elastic component which is the unmodified beam with the same wavelength as the primary beam, and a modified inelastic component, which has a longer wavelength [136]. Classical theory however, only predicts the unmodified beam [137].

The unmodified, elastic component is referred to as coherent scattering, and the
modified component as incoherent. However, this needs further qualifying. X-ray propagation can be described by Maxwell’s equations as free space coherent propagation of the radiation field. In matter, they induce a current which is linearly dependent upon the field strength, which can lead to interference effects of the scattered waves. The intensity of the field becomes re-distributed over space and time and multiple scattering leads to refraction phenomena. Since Maxwell’s equations describe coherent scattering, all scattering processes at the basic level can be viewed as intrinsically coherent. However, this intrinsic coherence may not necessarily result in observable interference, since experimental conditions of measurement will determine its probability [138]. X-ray production by synchrotrons and x-ray tubes, consist of many independent sources that have no correlation between phases, hence the average value of the interference term vanishes when squared for the intensity. Therefore coherence detection requires high spatial or temporal resolution measurement [138].

4.2.1 Classical scattering

Under the classical model proposed by Hendrik A. Lorentz (1909) and others, matter consisted of mass and charge. Each kind of charge was considered as a charge density $\rho$. These charges caused electrical fields, and moving charges produced a current density $\mathbf{J} = \rho \mathbf{v}$, where $\mathbf{v}$ is the velocity. In the spirit of classical physics, charge and current density could be subdivided indefinitely and each subdivision could be labelled and its motion followed. The positive and negative charges were modelled as small spheres with a radius of the order of the size of the nucleus, $10^{-15}$m, and the total charge was given by $Z$ times $e$. For the case of the negative charge, the elemental charge $e$ was called an electron, which maintains its separate identity at all times, and furthermore the positive and negative charges were independent and capable of moving through one another [139].
4.2.2 Dipole radiation

In the atomic model, the nucleus and associated electrons form a dipole that is acted upon by the incident radiation. Dynamical properties assigned to the model determine the various motions of the nucleus and electrons. Initially the electrons are considered at rest and to be rigidly attached to the nucleus with the excitation process consisting of these charges departing from their equilibrium positions under the influence of an external force such as a collision or incident radiation. Subsequent motion is then determined by Newton’s laws with the Coulomb force holding the charges together. Unfortunately, this model is insufficient to explain the character of the radiation emitted, and Lorentz made additional assumptions of a non-electrical nature to give qualitatively the correct predictions [136].

To arrive at a scattering theory that explains the refraction of x-rays that will be used in this thesis, it is necessary to trace the scattering theory from the simple dipole model, to the free electron, bound electron and many electrons models. Maxwell’s theory gives a means of calculating the electric and magnetic fields emanating from charges and currents, which in turn act upon them and influence their motions [139]. The equations of Maxwell for mediums that are continuous are

\[
\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} \\
\n\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \\
\n\nabla \cdot \mathbf{B} = 0 \\
\n\nabla \cdot \mathbf{D} = \rho
\]

where \( \mathbf{E} \) is the electric field vector, \( \mathbf{H} = \mu_0 \mathbf{B} \) is the magnetic field vector, \( \mathbf{D} = \epsilon_0 \mathbf{E} \) is the electric displacement, \( \mathbf{B} \) is the magnetic density, \( \mathbf{J} \) is the current density, \( \rho \) is the charge density, \( \epsilon_0 \) is the permittivity of free space, and \( \mu_0 \) is the magnetic permeability [5]. These equations relate the fields to the charges, which in turn relates the forces they exert on charges and the law of motion is determined by the influence of all acting
forces [139]. The law of motion is governed by Newton’s second law, and equated to the Lorentz force

\[ \mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \]  

(4.12)

Since \( |\mathbf{v}| \ll c \), the magnetic component can be neglected which leaves finding the electric component \( \mathbf{E} \). This can be done in a number of ways as for example by solving for the scalar \( \phi \) and vector potentials \( \mathbf{A} \) by

\[ \mathbf{E} = -\nabla \phi - \frac{\partial \mathbf{A}}{\partial t} \]  

(4.13)

\[ \mathbf{B} = \nabla \times \mathbf{A} \]

to obtain two second order, partial differential equations

\[ \nabla^2 \phi - \frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} = -\frac{\rho}{\epsilon_0} \]  

(4.14)

\[ \nabla^2 \mathbf{A} - \frac{1}{c^2} \frac{\partial^2 \mathbf{A}}{\partial t^2} = -\frac{\mathbf{J}}{\epsilon_0 c^2} \]

with the added condition [140] for the gauge, that

\[ \nabla \cdot \mathbf{A} = -\frac{q}{c^2} \frac{\partial \phi}{\partial t} \]  

(4.15)

Solutions for \( \phi \) and \( \mathbf{A} \) can be plane, cylindrical or spherical waves, but after some manipulation can be found to be

\[ \phi(1, t) = \int \rho(2, t - \frac{r_{12}}{c}) \frac{1}{4\pi\epsilon_0 r_{12}} dV_2 \]  

(4.16)

\[ \mathbf{A}(1, t) = \int \mathbf{J}(2, t - \frac{r_{12}}{c}) \frac{1}{4\pi\epsilon_0 r_{12}} dV_2 \]

where \( \phi(1, t) \) means the scalar field at point \((x_1, y_1, z_1)\) at time \(t\), due to a source point \(\rho(2, t - \frac{r_{12}}{c})\) at the position \((x_2, y_2, z_2)\) at an earlier time \(t - \frac{r_{12}}{c}\), and \(r_{12}\) is the distance between the two points. Substituting these back into Eq. 4.13 to obtain the electric
and magnetic fields, results in an equation for the electric field [140] as

\[ E = -\frac{q}{4\pi \epsilon_0} \left[ \hat{e}_{r'} \frac{r'}{r'^2} + \frac{r'}{c} \frac{d}{dt} \left( \frac{\hat{e}_{r'}}{r'^2} \right) + \frac{1}{c^2} \frac{d^2}{dt^2} \hat{e}_{r'} \right] \]  

(4.17)

where \( \hat{e}_{r'} \) is a unit vector of the charge position and \( r' \) is the position of the charge at the retarded time of \( t - \frac{r}{c} \). The first term is the Coulomb field and the second is a modification for finite time of transmission, while the third term as explained by Feynman [140] accounts for radiation. This can be expressed as an acceleration component

\[ \frac{d^2}{dt^2} \hat{e}_{r'} \bigg|_x = a_x(t - \frac{r'}{c}) \]  

(4.18)

Thus the field scattered due to the transverse component, \( a_T \), of an accelerating electron is

\[ E(r, t) = \frac{q}{4\pi \epsilon_0 c^2 r} a_T(t - \frac{r}{c}) \]  

(4.19)

To allow for finite time of transmission, the time \( t \) is modified to \( t - \frac{r'}{c} \). It can also be derived by an alternative method as given by Attwood [5] by forming a wave equation from Maxwell’s equations.

\[ \left( \frac{\partial^2}{\partial t^2} - c^2 \nabla^2 \right) E = -\frac{1}{\epsilon_0} \left[ \frac{\partial J}{\partial t} + c^2 \nabla \rho \right] \]  

(4.20)

and the equation of charge continuity

\[ \nabla \cdot J + \frac{\partial \rho}{\partial t} = 0 \]  

(4.21)

The current density can be written as the product of charge density and velocity

\[ J = qNv \]  

(4.22)

Then solving for the transverse component of the electric field via a Green’s type solution, of the form

\[ E = \frac{1}{(2\pi)^4} \int \int \int \int \mathbf{E}_{k\omega} e^{-i(\omega t - k \cdot r)} d\omega dk \]  

(4.23)
where the Fourier transform is defined as

$$f(r) = \frac{1}{(2\pi)^3} \int \int \int F(k)e^{ik\cdot r}dk$$

(4.24)

Performing a similar transform for $J$ and equating the appropriate coefficients, leads to

$$E(r, t) = \frac{qa_T(t - r/c)}{4\pi\epsilon_0 c^2 r}$$

(4.25)

which is the same as Feynman’s third term. Thus the scattered electric field radiation $E$ can be calculated once the motions of individual electrons are known, and the total field can be found via the principle of superposition. The motion of the electrons can be determined given some known form for the incident radiation field. The simplest case is an oscillatory incident field such as $E_i = E_0 e^{i\omega t}$. The radiated power density $S$, of an electron can be deduced via Poynting’s theorem which is

$$S = E \times H$$

(4.26)

Once the electric field $E$ is known, the magnetic field $H$ maybe calculated from Maxwell’s equation

$$H = \sqrt{\frac{\epsilon_0}{\mu_0}} k_0 \times E(r, t)$$

(4.27)

where $k_0$ is the direction of propagation of radiated energy per unit area. Substituting Eq. 4.27 into Poynting’s theorem Eq. 4.26 gives

$$S = \sqrt{\frac{\epsilon_0}{\mu_0}} |E|^2 k_0$$

(4.28)

and substituting for the electric field via Eq. 4.25 gives the instantaneous power per unit area radiated by an accelerated electron

$$S = \frac{q^2|a_T|^2}{16\pi^2\epsilon_0 c^3 r^2} k_0$$

(4.29)

For an angle $\Theta$ between the direction of acceleration $a_T$ and the observation direction
\( \mathbf{k}_0 \), so that \( |\mathbf{a}_T| = |\mathbf{a}| \sin \Theta \), the equation is modified to

\[
S = \frac{q^2 |\mathbf{a}|^2 \sin^2 \Theta}{16\pi^2 \epsilon_0 c^3 r^2} \mathbf{k}_0
\]  

(4.30)

Since the radiated power can be written as \( S = \frac{dP}{dA} \mathbf{k}_0 \), where the area \( dA = r^2 d\Omega \), then the power per unit solid angle is

\[
\frac{dP}{d\Omega} = \frac{q^2 |\mathbf{a}|^2 \sin^2 \Theta}{16\pi^2 \epsilon_0 c^3}
\]  

(4.31)

This equation gives the radiation pattern for the dipole radiator in terms of solid angle. The full power is found by integration over the area or a sphere where \( dA = r^2 d\Omega = r^2 \sin \Theta d\theta d\phi \) and is

\[
P = \frac{8\pi}{3} \left( \frac{q^2 |\mathbf{a}|^2}{16\pi^2 \epsilon_0 c^3} \right)
\]  

(4.32)

For sinusoidal motion, averaging over one cycle introduces a factor of \( \frac{1}{2} \) so that

\[
\bar{P} = \frac{1}{2} \frac{8\pi}{3} \left( \frac{q^2 |\mathbf{a}|^2}{16\pi^2 \epsilon_0 c^3} \right)
\]  

(4.33)

The scattering cross section \( \sigma \) is a measure of the power of an electron to scatter incident radiation and is given as an effective area for redirecting the incident radiation. It is defined \([5]\) as the average power radiated divided by the average incident power \( |\mathbf{S}_i| \)

\[
\sigma = \frac{\bar{P}_{\text{scattered}}}{|\mathbf{S}_i|}
\]  

(4.34)

It measures the ability of an object, such as an electron to remove photons from the incident beam and re-emit them in new directions. Thus there are scattering and absorption cross sections which are related to Eq. 4.2. The Thomson cross section can be derived as a natural consequence when the electron is considered free, whereas the case for a bound oscillator with an extra term for damping leads to Rayleigh scattering.
4.2.3 Scattering by a free electron - Thomson scattering

For low-intensity light, Thomson scattering is a linear process with no change to the frequency of the radiation [141]. This is an approximation in the low energy limit where quantum effects are no longer significant. For high intensity light e.g laser light, an electron may acquire relativistic velocities and emit radiation at higher harmonics of the light frequency and is called Nonlinear Thomson scattering. Applications for nonlinear scattering are new types of x-rays sources with applications such as angiography, which are currently being explored by Lau et al [142].

J. J. Thomson (1906) showed in cgs units, on the basis of classical theory, that when a beam of x-rays traverses matter it should be scattered by the scattering coefficient $\sigma$ or cross section which is given by

$$\sigma = \frac{8\pi}{3} \frac{e^4}{m^2c^4} N_e$$

(4.35)

where, $e$ and $m$ are the charge and mass of the electron respectively, $c$ is the velocity of light and $N_e$ is the number of electrons [136]. In modern mks units, where the charge of the electron conversion from cgs units is $e = \frac{q}{4\pi\varepsilon_0}$ [140] and for one electron, this is expressed as

$$\sigma = \frac{8\pi}{3} r_e^2$$

(4.36)

where $r_e = \frac{q^2}{4\pi\varepsilon_0 mc^2} = 2.82 \times 10^{-15} m$. Newton’s second law $F = ma$ is equated with the Lorentz force $F = -qE$. The acceleration of the electron due to the incident electric field $E_i$ is simpler than the dipole case with

$$a(r, t) = \frac{q}{m} E_i(r, t)$$

(4.37)

This accelerated motion in turn radiates energy according to Eq. 4.25, and again only the transverse component of this electric field to any observation point is important with $a_t = a \sin \Theta$, so substituting Eq. 4.37 into Eq. 4.25, and an oscillatory incident
field $E_i = E_i e^{-i\omega t}$, the radiated field is

$$E(r, t) = -\frac{q^2 E_i \sin \Theta}{4\pi \varepsilon_0 mc^2 r} e^{-i\omega(t - \frac{r}{c})}$$  \hspace{1cm} (4.38)$$

Using the classical electron radius $r_e$, this simplifies further to

$$E(r, t) = -\frac{r_e}{r} E_i \sin \Theta \ e^{-i\omega(t - \frac{r}{c})}$$  \hspace{1cm} (4.39)$$

where $t - r/c$ is the time delay of the radiated field. The average power emitted by this electric field is calculated from Eq. 4.33

$$P = \frac{1}{2} \frac{8\pi^3}{3} \left( \frac{q^4 |E_i|^2}{16\pi^2 \varepsilon_0 m^2 c^3} \right)$$  \hspace{1cm} (4.40)$$

The incident energy is found via Poynting’s theorem $S = E \times H$, so that the cross section is found by

$$\sigma = \frac{P_{\text{scattered}}}{|S_i|} = \frac{4\pi}{3} \left( \frac{q^4 |E_i|^2}{16\pi^2 \varepsilon_0 m^2 c^3} \right)$$  \hspace{1cm} (4.41)$$

where $|S_i| = \frac{1}{2} \sqrt{\mu_0 |E|^2 k_0}$ is the average incident energy for an oscillating field. After some rearranging this simplifies to

$$\sigma_e = \frac{8\pi}{3} r_e^2 = 6.65 \times 10^{-25} \ cm^2$$  \hspace{1cm} (4.42)$$

There is no frequency dependence for the Thomson cross section and it is assumed to be independent of the strength of the original light, and therefore a fundamental physical constant. The scattering cross section is the equivalent area of the incident wavefront which delivers the same power as that re-radiated by the particle, and hence is a proportionality constant, with dimensions of area \([139]\).

$$\sigma = \frac{\text{total re-radiated power}}{S}$$  \hspace{1cm} (4.43)$$

By analogy, the differential scattering cross section is the relative intensity by scattering
in different directions, the angular factor or \( \frac{d\sigma}{d\Omega} \), is defined as

\[
\frac{d\sigma}{d\Omega} = \frac{4\pi}{S} \frac{dP}{d\Omega}
\]  

For the case of a polarized incident beam in the same plane as the incident and scattered directions, with \( \theta \) the angle of observation to the polarization direction, this becomes [143]

\[
\frac{d\sigma}{d\Omega} = \left( \frac{q^2}{4\pi \epsilon_0 mc^2} \right)^2 \sin^2 \theta
\]  

If the polarization is at right angles then the equation is

\[
\frac{d\sigma}{d\Omega} = \left( \frac{q^2}{4\pi \epsilon_0 mc^2} \right)^2
\]  

Hence the differential scattering cross section for unpolarized incident radiation, expressed as the average between the two polarizations, is

\[
\frac{d\sigma}{d\Omega} = \left( \frac{q^2}{4\pi \epsilon_0 mc^2} \right)^2 \frac{1 + \cos^2 \phi}{2}
\]  

where \( \phi \) is the angle subtended between the direction of the incident radiation and that of the scattered radiation. The important point for x-rays is that the electrons are vibrating out of phase with the incoming radiation and furthermore the cross section is largely independent of frequency. The frequency independent term for the Thomson cross section is given by

\[
\left( \frac{d\sigma}{d\Omega} \right)_{Th} = f_{Th}(\phi) = \frac{1}{2} r_e^2 (1 + \cos^2 \phi)
\]

making \( \left( \frac{d\sigma}{d\Omega} \right)_{Th} \) of the order of \( 10^{-29} m^2/sr \).
4.2.4 Scattering by a single bound electron - Rayleigh scattering

Considering just one electron with discrete binding energy $\omega_s$ and complex damping coefficient $\gamma$, the equation of motion is [5]

$$m \left( \frac{d^2x}{dt^2} + \gamma \frac{dx}{dt} + \omega_s^2 x \right) = -q(E_i + v \times B_i) \approx 0$$

(4.49)

With the assumption of an oscillatory incident field, $E_i = E_0e^{-i\omega t}$, then the solution to this equation can be written in a similar oscillatory manner as $x = x_0e^{-i\omega t}$. Differentiating and substituting into the above equation results in a solution for position as a function of frequency as

$$x = \frac{1}{\omega^2 - \omega_s^2 + i\gamma\omega} \frac{qE_i}{m}$$

(4.50)

The acceleration is found by differentiating this twice

$$a = \ddot{x} = \frac{-\omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega} \frac{qE_i}{m}$$

(4.51)

The scattered electric field is found from Eq. 4.25. By calculating the incident power and the power radiated the cross section for a bound electron $\sigma_b$, from Eq. 4.41 can be deduced

$$\sigma_b(\omega) = \frac{8\pi}{3} r_e^2 \frac{\omega^4}{(\omega^2 - \omega_s^2)^2 + (\gamma\omega)^2}$$

(4.52)

This equation unlike the free electron Thomson case, has a frequency dependence which rises to a maximum, near the resonance frequency $\omega = \sqrt{\omega_s^2 \left( \frac{1}{2}\gamma^2 \right)}$ of

$$\sigma_b(\omega_s) = \frac{8\pi}{3} r_e^2 \frac{\omega_s^4}{\gamma^2 \omega_s^2} = \sigma_T \left( \frac{\omega_s}{\gamma} \right)^2$$

(4.53)
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For large $\omega \gg \omega_s$, and assuming the damping factor $\gamma$ is small, the cross section reduces to the Thomson case $\sigma_T$, where the oscillators are essentially free

$$\sigma_b(\omega) = \frac{8\pi}{3} e^2 \frac{\omega^4}{(\omega^2 - \omega_s^2)^2 + (\gamma \omega)^2}$$

(4.54)

$$\approx \frac{8\pi}{3} e^2 \frac{\omega^4}{\omega^2}$$

$$= \frac{8\pi}{3} e \frac{\omega^4}{\omega_s^2}$$

$$= \sigma_T$$

For small $\omega$ such that $\omega \ll \omega_s$ and $\gamma \ll \omega_s$, the cross section reduces to a form first determined by Lord Raleigh (1899) which has a strong $\omega^4$ dependence

$$\sigma_b(\omega) = \frac{8\pi}{3} e^2 \frac{\omega^4}{\omega_s^2} = \frac{8\pi}{3} e \left(\frac{\omega}{\omega_s}\right)^4$$

(4.55)

which is often used to explain the blue color of the sky, since blue light scatters about 16 times more than red light.

4.2.5 Scattering by a multi-electron atom

In the semi-classical model the electrons of a multi-electron atom can be given a charge distribution $\eta$ as a function of position and time of the form [5]

$$\eta(r, t) = \sum_{s=1}^{Z} \delta[r - \Delta r_s(t)]$$

(4.56)

where $\delta$ is the Dirac delta, and $\Delta r$ is the small displacement of each charge. Allowing the incident field to be more dominant on the electrons than effects from its neighbours, i.e. the Born approximation, this modifies the electric field from multi-electrons to

$$E(r, t) = \frac{q}{4\pi \varepsilon_0 c^2} \sum_{s=1}^{Z} \frac{a_T(t - r/c)}{r_s}$$

(4.57)
The incident electric field $E_i$ must be modified to account for the differing phase seen by each electron to $E_i(r, t) \rightarrow E_i e^{-i(\omega t - \mathbf{k} \cdot \Delta \mathbf{r}_s)}$. Solving the equation of motion results in an expression for the positions of the electrons as

$$x_s(t) = \frac{1}{\omega^2 - \omega_s^2 + i\gamma\omega} \frac{q}{m} E_i e^{-i(\omega t - \mathbf{k} \cdot \Delta \mathbf{r}_s)}$$  \hspace{1cm} (4.58)

Differentiating this twice gives the acceleration

$$a_s(t) = \ddot{x}_s = \frac{-\omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega} \frac{q}{m} E_i e^{-i(\omega t - \mathbf{k} \cdot \Delta \mathbf{r}_s)}$$  \hspace{1cm} (4.59)

Hence the electric field due to the multi-electron movement is the extension of Eq. 4.38

$$E(r, t) = -\frac{q^2}{4\pi\epsilon_0 mc^2} \sum_{s=1}^{Z} \frac{\omega^2 E_i \sin \Theta}{\omega^2 - \omega_s^2 + i\gamma\omega} \frac{1}{r_s} e^{-i[\omega(t - \frac{r}{c}) - \mathbf{k} \cdot \Delta \mathbf{r}_s]}$$  \hspace{1cm} (4.60)

where $r_s \equiv r - \Delta \mathbf{r}_s$ and $r_s = |\mathbf{r}_s|$ and for $r \gg \Delta \mathbf{r}_s$, to a good approximation $r_s \approx r - \mathbf{k}_0 \cdot \Delta \mathbf{r}_s$ so that the following expression holds true

$$E(r, t) = -\frac{q^2}{4\pi\epsilon_0 mc^2} \sum_{s=1}^{Z} \frac{\omega^2 E_i \sin \Theta}{\omega^2 - \omega_s^2 + i\gamma\omega} \frac{1}{r_s} \exp \left\{ -i \left[ \omega \left( t - \frac{r}{c} \right) + \left( \mathbf{k} - \mathbf{k}_0 \right) \cdot \Delta \mathbf{r}_s \right] \right\}$$  \hspace{1cm} (4.61)

where $\mathbf{Q} = \mathbf{k} - \mathbf{k}_0$ is the scattering vector. Its magnitude $|\mathbf{Q}| = 2k_i \sin \theta$, where $2\theta$ is the scattering angle between $\mathbf{k}$ and $\mathbf{k}_0$. Using this expression for $\mathbf{Q}$, the electric field becomes

$$E(r, t) = -\frac{r_e}{r} \sum_{s=1}^{Z} \frac{\omega^2 e^{-i\mathbf{Q} \cdot \Delta \mathbf{r}_s}}{\omega^2 - \omega_s^2 + i\gamma\omega} E_i \sin \Theta e^{-i\omega(t - \frac{r}{c})}$$  \hspace{1cm} (4.62)

The function $f(\mathbf{Q}, \omega)$ is called the complex scattering factor

$$f(\mathbf{Q}, \omega) = \sum_{s=1}^{Z} \frac{\omega^2 e^{-i\mathbf{Q} \cdot \Delta \mathbf{r}_s}}{\omega^2 - \omega_s^2 + i\gamma\omega}$$  \hspace{1cm} (4.63)
The scattered electric field from a multi-electron atom may now be written with the complex scattering factor as

\[ E(r, t) = -\frac{r_e}{r} f(Q, \omega) E_i \sin \Theta e^{-i\omega(t - \frac{r}{c})} \] (4.64)

The differential and total cross sections may also be written as

\[
\frac{d\sigma(\omega)}{d\Omega} = r_e^2 |f|^2 \sin^2 \Theta \quad (4.65)
\]

\[
\sigma(\omega) = \frac{8\pi}{3} r_e^2 |f|^2 \quad (4.66)
\]

### 4.2.6 Atomic scattering factors

The atomic form factor or scattering factor includes the explicit phase variation \( e^{i\phi_s} = e^{-i\omega \Delta k \cdot \Delta r} \) for each of the electrons in the atom. This factor does not in general simplify except for two special cases. The long wavelength limit and the forward scattering case. Now the magnitude of \( Q \) is \( |Q| = 2k_i \sin \theta \), and since \( k_i = \frac{2\pi}{\lambda} \), then \( Q = |Q| = \frac{4\pi}{\lambda} \sin \theta \).

By making the assumption that the charge distribution is contained within some finite radius, say the Bohr radius \( a_0 \), the phase term for \( f \) is bounded by

\[
|Q \cdot \Delta r| \leq \frac{4\pi a_0}{\lambda} \sin \theta \quad (4.67)
\]

For the two special cases:

\[
|Q \cdot \Delta r| \rightarrow 0 \quad \text{for } a_0/\lambda \ll 1 \quad \text{(long wave length limit)} \quad (4.68)
\]

\[
|Q \cdot \Delta r| \rightarrow 0 \quad \text{for } \theta \ll 1 \quad \text{(forward scattering)}
\]

The atomic scattering factor reduces to

\[
f^0(\omega) = f(Q, \omega) = \sum_{s=1}^{Z} \frac{\omega^2}{\omega^2 - \omega_s^2 + i\gamma} \quad (4.69)
\]
One more generalization is required for multiple resonances by the introduction of oscillator strengths $g_s$, with the condition that the sum of the oscillator strengths equals the number of electrons

$$
\sum_s g_s = Z \tag{4.70}
$$

These oscillator strengths arise as the transition probabilities between states $\psi_k$ and $\psi_s$ summed over final states $n$ from an initial state $k$ and must be calculated from quantum mechanics

$$
\sum_{s,n} g_{n,s} = Z \tag{4.71}
$$

So that the atomic scattering factor is now written as

$$
f^0(\omega) = f(Q, \omega) = \sum_s \frac{g_s \omega^2}{\omega^2 - \omega_s^2 + i\gamma} \tag{4.72}
$$

where the superscript $^0$ indicates one of the two conditions in Eq. 4.68 applies. In the limit as $\lambda/a_0 \gg 1$, ie long wave length limit, the scattering factor reduces to

$$
f(Q, \omega) \rightarrow f^0(\omega) \rightarrow \sum_s g_s = Z \tag{4.73}
$$

This equation was once used as a method to determine the number of electrons per atom in a material and was one of the ways in which scattering theory played an important role the development of early atomic theory [136]. The differential scattering cross section becomes

$$
\frac{d\sigma}{d\Omega} = Z^2 r_e^2 \sin^2 \Theta = Z^2 \frac{d\sigma_T}{d\Omega} \tag{4.74}
$$

and total cross section

$$
\sigma(\omega) = \frac{8\pi}{3} r_e^2 Z^2 = Z^2 \sigma_e \tag{4.75}
$$

where $\sigma_e$ is scattering from one electron. Therefore in a similar fashion to attenuation or absorption, the scattering process reduces the intensity of the incident beam via

$$
I = I_0 e^{-\sigma \rho z} \tag{4.76}
$$
where $\rho$ is the number density of scatterers. Experimentally, the cross section $\sigma$, can be deduced by measuring $I_0$, $I$ and $z$, with the assumption that only scattering processes remove energy from the beam. Once $\sigma$ is known, the number of electrons $n$ per cubic centimeter of scattering material can then be calculated. Charles Glover Barkla (1911) was one of the first to do this and determine the number of electrons per atom [144].

### 4.3 Refractive index

The deviations from unity are so small $\sim 10^{-6}$ for the refractive index of many materials at x-ray energies, that the forward scattering limit applies, and the atomic scattering factor $f$ is written as $f^0$, and can be further written as $f^0(\omega) = f^0_1(\omega) - i f^0_2(\omega)$ [5]. Sellmeier (1870) determined a formula for refraction based on the elastic solid theory of light for multiple oscillators as

$$ n^2 = 1 + \frac{e^2}{\pi m} \sum_i \frac{N_i}{\omega_{0i}^2 - \omega^2} $$

where $N$ is the number of electrons per unit volume, and $\omega_{0i}$ are the natural frequencies. For a gas, the refractive index equation is modified to include the damping constant [140]

$$ n^2 = 1 + \sum N_K \frac{\left( \frac{\phi^2}{m\epsilon_0} \right)}{2(-\omega^2 + i\gamma_k \omega + \omega_k^2)} $$

However, for dense materials, the electric field is modified by the inclusion of a polarizability term $p = \alpha E$, where $\alpha(\omega)$ is the polarizability so that the refractive index is

$$ n^2 = 1 + \frac{N\alpha}{1 - \frac{N\alpha}{3}} $$

For a plate of material consisting of $N$ identical dipole oscillators, Feynman calculates the electric field $E(P)$ to be proportional to $i\omega x_0 e^{i\omega(t-z/c)}$, the velocity of the charges


\[ E(P) = -\frac{\eta q}{2\epsilon_0 c} i \omega x_0 e^{i\omega(t-z/c)} \]  

(4.80)

\[ (\frac{\partial^2}{\partial t^2} - c^2 \nabla^2) \mathbf{E}_T(r, t) = -\frac{1}{\epsilon_0} \frac{\partial \mathbf{J}_T(r, t)}{\partial t} \]  

(4.82)

Attwood uses the transverse wave equation

\[ \frac{\partial^2}{\partial t^2} \mathbf{E}_T(r, t) = -\frac{1}{\epsilon_0} \frac{\partial \mathbf{J}_T(r, t)}{\partial t} \]  

(4.82)

which for forward scattering reduces to finding the special case of

\[ \mathbf{J}_0(r, t) = -e n_a \sum_s g_s v_s(r, t) \]  

(4.84)

since electrons and similar atoms all contribute identically, and \( n_a \) is average density of atoms. Substituting this into the wave equation

\[ \frac{\partial^2}{\partial t^2} \mathbf{E}_T(r, t) = -\frac{e^2 n_a}{\epsilon_0 m} \sum_s \frac{g_s}{(\omega^2 - \omega_s^2) + i\gamma \omega} \frac{\partial^2 \mathbf{E}(r, t)}{\partial t^2} \]  

(4.85)

rearranging this so terms are combined with similar operators

\[ \left[ 1 - \frac{e^2 n_a}{\epsilon_0 m} \sum_s \frac{g_s}{(\omega^2 - \omega_s^2) + i\gamma \omega} \right] \frac{\partial^2}{\partial t^2} \mathbf{E}(r, t) = 0 \]  

(4.86)

which can be simplified with the introduction of the complex refractive index \( n(\omega) \) to

\[ \left[ \frac{\partial^2}{\partial t^2} - c^2 n^2(\omega) \nabla^2 \right] \mathbf{E}_T(r, t) = 0 \]  

(4.87)
with

\[ n(\omega) = \sqrt{1 - \frac{e^2 n_a}{\epsilon_0 m} \sum \frac{g_s}{(\omega^2 - \omega_s^2) + i\gamma_s\omega}} \]  

(4.88)

This can be further simplified for x-rays to

\[ n(\omega) = 1 - \frac{e^2 n_a}{2 \epsilon_0 m} \sum \frac{g_s}{(\omega^2 - \omega_s^2) + i\gamma_s\omega} \]  

(4.89)

Using the classical radius \( r_c \) and the definition of \( f^0 = f^0_1(\omega) - i f^0_2(\omega) \) the refractive index \( n(\omega) \) becomes

\[ n(\omega) = 1 - \frac{n_a r_c \lambda^2}{2\pi} \left[ f^0_1(\omega) - i f^0_2(\omega) \right] \]  

(4.90)

Which is commonly expressed as \( n(\omega) = 1 - \delta + i\beta \) so that

\[ \delta = \frac{n_a r_c \lambda^2}{2\pi} f^0_1(\omega) \]  

(4.91)

\[ \beta = \frac{n_a r_c \lambda^2}{2\pi} f^0_2(\omega) \]  

(4.92)

The refractive index expressed as \( n(\omega) = 1 - \delta + i\beta \) is the common form among the electrodynamics and optical sciences community, where as \( n(\omega) = 1 - \delta - i\beta \) is the form used by the x-ray community. The sign depends on the form the waves are expressed \( \exp[i(\omega t - kr)] \) in the case of \(-i\beta \) and \( \exp[-i(\omega t - kr)] \) in the case of \(+i\beta \) and are equivalent, see Attwood [5]. Henke et al [145], provide tables of atomic scattering factors based upon photoabsorption measurements of elements in their elemental state. These are based on a compilation of the available experimental measurements and theoretical calculations. Some elements in the tabulations rely on theoretical calculations and interpolations across \( Z \). For large energies (i.e. x-ray range) and above the K absorption edge \( f^0_1 \rightarrow Z \). An example for of \( f^0_1, f^0_2 \) and \( \mu \) for carbon is given in Fig. 4.7.
4.4 Inelastic scattering

Classical theory was unable to explain the modified beam in scattering experiments [147]. Arthur Compton (1921) showed that the Thomson cross section with respect to energy, was not constant due to quantum mechanical effects [136]. His discovery of the Compton effect, enabled a definite value for the classical electron radius $r_e$ to be calculated. Compton (1923) and Peter Debye (1923) independently derived a relationship [147] between the wavelength and the scattering angle of radiation softened by scattering from stationary, free electrons as

\[
(h\nu_f)^{free} = \frac{h\nu_i}{1 + \frac{h\nu_i}{mc^2}(1 - \cos \theta_f)}
\]  

(4.93)
The observed experimental data from solid data was not a one to one correspondence between angle and energy, which led Compton to hypothesize that the electrons were not stationary. Klein and Nishina (1929) applied relativistic quantum theory to derive an expression for the differential cross section as

$$\frac{d\sigma}{d\Omega_f} = \frac{r_e^2}{2} \left( \frac{(h\nu_f)^{\text{free}}}{h\nu_i} \right)^2 \left( \frac{(h\nu_f)^{\text{free}}}{h\nu_i} + \frac{h\nu_i}{(h\nu_f)^{\text{free}} - \sin^2 \theta_f} \right)$$

(4.94)

For \((h\nu_f)^{\text{free}} \approx h\nu_i\), this equation reduces to the Thomson result. When the electron is bound, the process is defined as incoherent and inelastic [147]. For the case where there is scattering with excitation, it is referred to as Raman scattering, whereas for scattering with ionization it is called Compton scattering. The description of Compton scattering is simplified with the use of the Independent Particle Model (IPA), where scattering occurs from an electron in a particular subshell, and the initial state consists of a photon and bound electron. Calculations of scattering are dependent on the energy and polarization of the photon plus the energy level and magnetic sub-state of the bound electron [147]. The final state consists of the ejected electron, a scattered photon and an excited ion which may relax to the ground state via fluorescence or Auger emission.

### 4.5 Scatter modelling

For x-ray imaging modalities such as bone densitometry, angiography, CT as well as conventional radiography, both inelastic and elastic scatter interfere with diagnostic information by changing the spatial information or changing the energy of the beam or by adding noise. Ideally the interaction would be such that the photon would either be photoelectrically absorbed or not interact at all, rather than being deviated off course. The amount of scatter increases with beam area and target thickness so that for example, in chest radiographs, around the mediastinum, scatter can be as much as 90 percent of the radiation reaching the detector. Traditional use of scatter reduction
grids only reduces this to 50-60% [148]. Therefore much effort has been invested to overcome these limitations [149].

As well as x-ray scatter within the patient, there may also be further light scatter within the detector, known as veiling glare. Ways of dealing with scatter and glare can be divided into two methods: preventative and corrective. Preventative methods such as air gaps, grids, scanning slot devices etc., use devices positioned before the detector. Some novel developments are an antiscatter collimator by Endo et al [150], for cone beam CT, which is comprised of thin equally spaced molybdenum (Mo) blades with sufficient longitudinal length and pitch to cover the detector, that can be adjusted for concentration to the x-ray focal spot. Ning et al [151] use a hybrid technique using air gaps and an anti-scatter grid plus a scatter correction algorithm for the remaining residual scatter.

The corrective methods usually require some type sampling of scatter, and/or a model by which to make the corrections. Sampling of scattered radiation by Pb blockers has been in use since 1921 when Wilsey [133] used them to measure the scatter to primary ratio (SPR). By positioning a small amount of Pb, usually a square or a disc on the entrance side of the object, so that the primary beam \( (P) \) is absorbed, sampling in its shadow gives a measure of the scattered radiation \( (S) \). Removing the object, it is also possible to measure any diffuse or off focal radiation, however this has been shown to be very minor [133]. By using an array of such sampling Pb absorbers, the scatter may estimated by interpolating between the samples [152]. This requires two exposures, one with the arrays (to get \( S \)) and one without (to get \( S + P \)) so that subtraction, gives a measurement of the amount of scatter. The converse can also be done, that is using by an array of apertures in a Pb sheet. This measures the primary radiation \( (P) \) only, which results in less dose to the patient, then another without the apertures to get \( S + P \) [153].

Of theoretical approaches, one is the use of linear systems theory, which treats the image as a convolution of the scatter and primary information. Examples of
its implementation are by Shaw et al [154] who used a rectangular blurring kernel convolved with the image as an estimate of the scatter. Naimuddin et al [155] used a similar method but with a weighting factor dependent on the image intensity. Love and Kruger [156] used a double exponential for the kernel scatter point spread function while Seibert et al [157] used a rotationally symmetric invariant point spread function.

The approach that will be followed here is known as the scatter generation model. An example of this by Aus et al [158], is an estimate of the amount of incoherent scatter and induced fluorescence, generated on a fractional basis on an arbitrary irradiated object, using the photoelectric absorption cross section $\tau$, incoherent cross section $\sigma$ and the linear attenuation coefficient $\mu$, is

$$
\left( \frac{S}{P} \right)_{\text{total}} = \sum_i (F_S)_i^* \left[ P_\alpha \frac{\tau(E_P)}{\mu(E_P)} \right]_i + \sum_j (F_S)_j^* \left[ \frac{\sigma(E_P)}{\mu(E_P)} \right]_j \quad (4.95)
$$

where $F_S$ is related to the fraction of total number of primary photons for each energy region, $Y$ is the fluorescence yield, and $P_\alpha$ is the probability of K or L shell interaction.

A more comprehensive model is provided by Inanc [159], which is designed to be used as a radiographic simulation code, with comparisons to existing codes, such as XRSIM, RADICAD, SINDBAD. His method is based on a deterministic integral transport equation

$$
I(r, E, \Omega) = \int_0^{R_T} q(r - R'\Omega, E, \Omega) e^{-\int_0^{R'} \Sigma_t(r - R''\Omega, E) dR''} dR' + I(r_\Gamma, E, \Omega) e^{-\int_0^{R_T} \Sigma_t(r - R''\Omega, E) dR''}
$$

where $I(r, E, \Omega)$ is the angular photon flux, $q(r - R'\Omega, E, \Omega)$ is the angular scattered photon flux, $r$ is the vector position $(x, y, z)$, $r_\Gamma$ is the object boundary, $E$ is the photon energy, $\Omega$ is the direction vector, $R$ is the path length along a direction vector, $R_\Gamma$ is the photon path length from the object boundary and $\Sigma_t$ is the total macroscopic cross
section i.e. the summation of the photoelectric absorption, coherent and incoherent cross sections. The scattering function $q$ is an integral over the energy and direction

$$q(r, E, \Omega) = \int_{4\pi} \int_{E}^{\infty} \Sigma(r, E' \rightarrow E, \Omega' \rightarrow \Omega) I(r, E', \Omega') \ d\Omega' dE' \quad (4.97)$$

where $\Sigma(r, E' \rightarrow E, \Omega' \rightarrow \Omega)$ represents the coherent and incoherent cross sections.

In the next section, a much simpler model to describe scatter is presented that depends only on the scattering angle and the distance to the detector, with no distinction as to the type of scatter.

### 4.5.1 A simple model of x-ray scatter

Previously developed as part of a Master’s thesis [3], a model was derived to estimate the amount of scatter arriving at the center of a detector from a scattering object. A schematic for the case of a point source geometry is shown in Fig. 4.8. It arose from measurements of scattered radiation made in the shadow of a Pb beam stopper, placed at the center on the tube side of the object. It was observed that the magnitudes of these measurements were dependent on the size of the disc, since the disc obscures possible scattering sites, so the model was used to back extrapolate to zero disc size. For simplicity, each elemental volume or voxel of the three dimensional homogeneous material was assumed to scatter isotropically with unit scattering strength. This a reasonable assumption when multiple scatter is involved without the bookkeeping as described in the model by Inanc. The derived equation for plane wave illumination, without attenuation was derived on purely geometric grounds based on the differential angle subtended by each scattering element or voxel as

$$h_{\text{disc}}(0, 0) = \int_{z=0}^{t} \int_{r=c}^{f_s} \int_{\phi_1}^{\phi_2} \frac{r(z + a)}{4\pi[r^2 + (z + a)^2]^{3/2}} dr d\phi' dz \quad (4.98)$$
Figure 4.8: Illustration of scatter reaching the detector from a scattering site
where \( t \) is the thickness of the scatterer, \( c \) is the radius of the Pb disc, \( f_s \) is the field size and \( \phi \) is the subtended angle, which for circular symmetry \( \phi_1 = 0 \) and \( \phi_2 = 2\pi \) reduces the equation to

\[
h_{disc}(0, 0) = \frac{1}{2} \int_{z=0}^{t} \int_{r=c}^{f_s} \frac{r(z + a)}{\sqrt{r^2 + (z + a)^2}^{3/2}} dr dz \tag{4.99}
\]

This represents the sum of all elements, assumed to scatter radiation isotropically and equally, arriving at the center of a two dimensional detector with polar coordinates \((0, 0)\).

Using tables of integration

\[
\int \frac{x}{(x^2 + a^2)^{3/2}} dx = -\frac{1}{\sqrt{x^2 + a^2}} \tag{4.100}
\]

This integral becomes

\[
h(0, 0) = \frac{1}{2} \int_{z=0}^{t} \int_{r=c}^{f_s} \frac{r(z + a)}{\sqrt{r^2 + (z + a)^2}^{3/2}} dr dz
\]

\[
= \frac{1}{2} \int_{z=0}^{t} \left[ \frac{z + a}{\sqrt{r^2 + (z + a)^2}} \right]_{r=c}^{f_s} dz
\]

\[
= \frac{1}{2} \int_{z=0}^{t} \left[ -\frac{z + a}{\sqrt{f^2 + (z + a)^2}} + \frac{z + a}{\sqrt{c^2 + (z + a)^2}} \right] dz
\]

\[
= \frac{1}{2} \int_{u=a}^{t+a} \left[ -\frac{z + a}{\sqrt{f^2 + u^2}} + \frac{z + a}{\sqrt{c^2 + u^2}} \right] du
\]

\[
= \frac{1}{2} \left[ -\sqrt{f^2 + (t + a)^2} + \sqrt{c^2 + (t + a)^2} + \sqrt{a^2 + f^2} - \sqrt{a^2 + c^2} \right] \tag{4.102}
\]

This simple equation can be used to compare qualitatively, the variation of measured scatter with the disc size to arrive at a value for the extrapolated signal. For the purposes of this thesis, it was extended to calculate the scatter to all points at the detector, thereby broadening its usefulness. The details are derived and presented here as a possible mechanism of phase contrast loss by scattering from either the filter or
object.

Consider the contribution of volume element situated at \( r(r, \phi, z) \), to detector element situated at \( q(q, \psi) \) as depicted in Figs 4.8 and 4.9. This value is dependent upon the distance \( R \) and angle \( \theta \) to the detector. If the vector \( q \) is projected onto \( r \) plane, it is possible to draw the triangle \( \Delta ABC \) which enables \( R \) and \( \theta \) to be written in terms of the length \( AB, z \) and \( a \). The length \( AB \) is the difference of \( r \) and \( q \), projected onto the same plane.

\[
|AB| = |r - q| = \sqrt{(r \cos \phi - q \cos \psi)^2 + (r \sin \phi - q \sin \psi)^2}
\]

By pythagoras

\[
R = \sqrt{(r \cos \phi - q \cos \psi)^2 + (r \sin \phi - q \sin \psi)^2 + (z + a)^2} \quad (4.103)
\]

and the cosine of the angle \( \theta \) can be written

\[
\cos \theta = \frac{z + a}{\sqrt{(r \cos \phi - q \cos \psi)^2 + (r \sin \phi - q \sin \psi)^2 + (z + a)^2}} \quad (4.104)
\]

Therefore the total contribution of all scattering elements to an arbitrary detector point is

\[
h(q, \psi) = \int_{z=0}^{t} \int_{\phi=0}^{2\pi} \int_{r=a}^{c} \frac{r(z + a)}{[(r \cos \phi - q \cos \psi)^2 + (r \sin \phi - q \sin \psi)^2 + (z + a)^2]^{3/2}} dr d\phi dz \quad (4.105)
\]

This results in a relatively simple equation for a quick and easy calculation for the distribution of scatter for given object, given the field size, thickness and type of object and the air gap distance to the detector, the details of which are given in the next section.

The effects of attenuation may be included by considering the path length through
the object. For a diverging beam as shown in Fig. 4.9 the attenuation for the primary beam is $e^{-\mu l}$, where $l$ is the distance travelled through the object. The attenuation of the scattered beam is $e^{-\mu L}$, where $L$ is the distance the scattered beam travels through the object. Therefore Eq. 4.105 is modified to

$$h(q, \psi) = \int_{z=0}^{l} \int_{\phi=0}^{2\pi} \int_{r=c}^{s} \frac{r(z + a)e^{-\mu l}e^{-\mu L}}{[(r \cos \phi - q \cos \psi)^2 + (r \sin \phi - q \sin \psi)^2 + (z + a)^2]^{3/2}} dr d\phi dz$$

(4.106)
4.5.2 Evaluation of scatter

The evaluation of the expression including attenuation must be done numerically whereas the evaluating the expression without attenuation is particularly straightforward. Starting with

\[ h(q, \psi) = \int_{z=0}^{t} \int_{\phi=0}^{2\pi} \int_{r=c}^{f_s} \frac{r(z + a)}{[(r \cos \phi - q \cos \psi)^2 + (r \sin \phi - q \sin \psi)^2 + (z + a)^2]^{3/2}} drd\phi dz \]  

(4.107)

some simplification can be done by using an equivalent formulation

\[ h(q, \psi) = \int_{z=0}^{t} \int_{\phi=0}^{2\pi} \int_{r=c}^{f_s} \frac{r(z + a)}{[r^2 + q^2 - 2rq \cos(\psi - \phi) + (z + a)^2]^{3/2}} drd\phi dz \]  

(4.108)

It can be seen that the \( z \) integration is the easiest to carry out, thus rearranging Eq. 4.108

\[ h(q, \psi) = \int_{\phi=0}^{2\pi} \int_{r=c}^{f_s} \int_{z=0}^{t} \frac{(z + a)}{[r^2 + q^2 - 2rq \cos(\psi - \phi) + (z + a)^2]^{3/2}} dz \ r dr d\phi \]  

(4.109)

\[ = - \int_{\phi=0}^{2\pi} \int_{r=c}^{f_s} \int_{z=0}^{t} \frac{dz}{[r^2 + q^2 - 2rq \cos(\psi - \phi) + (z + a)^2]^{1/2}} \left[ \frac{1}{r} \right] \int_{z=0}^{t} \frac{dz}{[r^2 + q^2 - 2rq \cos(\psi - \phi) + (z + a)^2]^{1/2}} \ r dr d\phi \]  

\[ = - \int_{\phi=0}^{2\pi} \int_{r=c}^{f_s} \left[ \frac{r}{[r^2 + q^2 - 2rq \cos(\psi - \phi) + (z + a)^2]^{1/2}} \right] \int_{z=0}^{t} \frac{dz}{[r^2 + q^2 - 2rq \cos(\psi - \phi) + (z + a)^2]^{1/2}} \ r dr d\phi \]  

Using tabled identities

\[ \int_{(ax^2 + bx + c)^{1/2}} dx = \frac{1}{a} (ax^2 + bx + c)^{1/2} - \frac{b}{2a} \int_{(ax^2 + bx + c)^{1/2}} dx \]  

(4.110)
and

\[ \int \frac{1}{(ax^2 + bx + c)^{1/2}} \, dx = \frac{1}{a^{1/2}} \ln \left| 2a^{1/2}(ax^2 + bx + c)^{1/2} + 2ax + b \right| \]  

(4.111)

Setting \( a = 1, \ b = -2q \cos(\psi - \phi), \) and \( c_1 = q^2 + (t + a)^2, \) and \( c_2 = q^2 + a^2 \)

\[
h(q, \psi) = \int_{\phi=0}^{2\pi} \int_{r=c}^{r=r} \left[ \frac{r}{[r^2 + q^2 - 2rq \cos(\psi - \phi) + a^2]^{1/2}} - \frac{r}{[r^2 + q^2 - 2rq \cos(\psi - \phi) + (t + a)^2]^{1/2}} \right] \, dr \, d\phi
\]

\[
= \int_{\phi=0}^{2\pi} (f^2 + bf + c_1)^{1/2} - \frac{b}{2} \ln \left| 2(f^2 + bf + c_1)^{1/2} + 2f + b \right|
\]

\[
- (f^2 + bf + c_2)^{1/2} + \frac{b}{2} \ln \left| 2(f^2 + bf + c_2)^{1/2} + 2f + b \right|
\]

\[
- (c^2 + bf + c_1)^{1/2} - \frac{b}{2} \ln \left| 2(c^2 + bc + c_1)^{1/2} + 2c + b \right|
\]

\[
- (c^2 + bc + c_2)^{1/2} + \frac{b}{2} \ln \left| 2(c^2 + bc + c_2)^{1/2} + 2c + b \right| \, d\phi
\]

upon substituting for \( b, \ c_1 \) and \( c_2 \) this becomes

\[
h(q, \psi) = \int_{\phi=0}^{2\pi} \left[ \sqrt{f^2 - 2q \cos(\psi - \phi)f + q^2 + (t + a)^2}
\]

\[
+ q \cos(\psi - \phi) \ln \left| 2\sqrt{f^2 - 2q \cos(\psi - \phi)f + q^2 + (t + a)^2} + 2f - 2q \cos(\psi - \phi) \right|
\]

\[
- \sqrt{f^2 - 2q \cos(\psi - \phi)f + q^2 + a^2}
\]

\[
- q \cos(\psi - \phi) \ln \left| 2\sqrt{f^2 - 2q \cos(\psi - \phi)f + q^2 + a^2} + 2f - 2q \cos(\psi - \phi) \right|
\]

\[
- \sqrt{c^2 - 2q \cos(\psi - \phi)c + q^2 + (t + a)^2}
\]

\[
+ q \cos(\psi - \phi) \ln \left| 2\sqrt{c^2 - 2q \cos(\psi - \phi)c + q^2 + (t + a)^2} + 2c - 2q \cos(\psi - \phi) \right|
\]

\[
- \sqrt{c^2 - 2q \cos(\psi - \phi)c + q^2 + a^2}
\]

\[
- q \cos(\psi - \phi) \ln \left| 2\sqrt{c^2 - 2q \cos(\psi - \phi)c + q^2 + a^2} + 2c - 2q \cos(\psi - \phi) \right| \, d\phi
\]

The three integrals have been reduced to a simple, if long, equation. Examples of three dimensional images calculated using Matlab for a variety of parameters are shown in
Figure 4.10: Simulated scatter images for over area detector $h(q, \psi)$, with variations: top row, radius increasing, middle row, object thickness increasing and bottom row, air gap increasing.

Fig. 4.10. If attenuation is significant, then this expression is limited, but for small objects such as fibres or thin filters, then this equation may be used as an upper bound for scattered radiation reaching the detector.

### 4.5.3 Summary

This chapter has covered the basics of scattering theory, including attenuation, absorption, elastic and inelastic scattering. Building on the classical theory of elastic scattering, a foundation has been built for the complex refractive index $n = 1 - \delta + i\beta$, including useful formulae for the real and imaginary parts that will be used for calculations in the simulation chapters. In order to study phase contrast with minimal interference from absorption contrast and inelastic scatter, thin objects and filters are chosen so that elastic scatter dominates the interaction and its effects may consequently
be modelled and simulated.

In the range of energies used for diagnostic imaging, inelastic scatter and absorption contrast become increasingly important when the thickness of biological materials increases, which unfortunately is the case in medical diagnostic practice. These effects have been modelled with a simple model which will be tested in the next chapter. However the bulk of the thesis is reliant upon modelling elastic scattering by both diffraction and refraction.
Chapter 5

Experimental preliminaries

This chapter describes the experimental set up and the preliminary experiments needed to characterize the system. It describes the source, and the detectors used to capture images, the input/output relationship and the reproducibility of the system.

Various objects are tested for suitability to measure phase contrast including edges of different materials, step wedges, grooves, solid and hollow fibres. Of these, the Cuprophan RC55 dialysis fibre was ultimately chosen as the best test object showing phase contrast with virtually no absorption. However, the straightness of a fibre was difficult to control, therefore a software based fibre straightening program was written and used to obtain better and more consistent measurements.

The previous chapter developed a model of x-ray scatter which was tested in various formats in this chapter. Scatter from the filter was investigated but found to have negligible effect on phase contrast measurements as long as it was positioned far from the detector. Scatter from the enclosure however, did have a measurable effect on the image which is described here.
Figure 5.1: X-ray image of Gold mask test object used for source focussing

5.1 Equipment

5.1.1 X-ray source

The experiments were conducted at CSIRO, Materials Science and Engineering (CMSE). The micro-focus x-ray source was a Feinfocus Röntgen-Systeme, model FXE 225-20 with a tungsten target, and a minimum focal spot size of 4 microns. This has sufficient spatial coherence for phase contrast to be detected with a variety of detector types such as x-ray film, CCD camera or an image plate. Its focal spot size may be adjusted via the tube current setting. At each tube potential, the beam focus may be altered by controllable settings and checked visually by inspection of an image of a gold mask test object with measurable line pairs see Fig. 5.1.
5.1.2 X-ray detection

The detection of x-rays was accomplished by storage phosphor image plates, Fuji FDL-URV, although X-ray film and a charge coupled device (CCD) camera were also used. X-ray film has excellent resolution due to its relatively small thickness but has low sensitivity. Its dynamic range is limited to about 2 or 3 orders of magnitude [160].

Film-screen combinations are commonly used in medicine to improve sensitivity by absorbing more x-rays by the phosphor material in an intensifying screen. The phosphor converts x-rays to visible light via photoluminescence, but the gain in sensitivity is made at the expense of resolution. For this thesis, resolution and reproducibility were more important for phase contrast detection and therefore intensifying screens were not used. However, the main disadvantage of film is its lack of reproducibility since temperature and concentration of the developer affect its HD (Hurter and Driffield) curve. Furthermore, the conversion to digital format requires calibrated optical devices which were not readily available.

For the practicality of imaging with good resolution and reproducibility, image plates were preferred for image detection. Image formation is achieved by a radiation induced photostimulable luminescence (psl) process, in contrast to the photoluminescence process used by intensifying screens. The absorption material consists of tiny crystals (∼5 µm) of barium fluorobromide, which upon absorption of x-ray photons generates electron-hole pairs in very close proximity to the absorption site which in turn creates the latent image [160]. There are also trace amounts of bivalent europium that serve as a luminescence center (BaFBr: Eu2+) which are stimulated later by the dedicated scanner system using a HeNe laser [161]. For the experiments described in this thesis, a Fuji BAS 5000 scanner was used, capable of 25 and 50 µm scans. For a schematic of the scanning process see Fig. 5.2. Further technical information about the different types of image plates can be found in Munekawa [162].
The BAS 5000 digitizes the image plates from quantization levels (QL) to psl values via the formula

$$\text{psl} = \left(\frac{P_{\text{size}}}{100}\right)^2 \times \frac{4000}{s} \times 10^{L\left(\frac{Q_L}{2^{16}} - \frac{1}{2}\right)}$$  \hspace{1cm} (5.1)

where \(s\) is the sensitivity, set to 4000, \(L\) is the latitude, which set to 4, gives a range of 4 orders of magnitude.

To view these images, the software by Analytical Imaging Station (AIS\textsuperscript{TM}) was used for initial cursory analysis but since the analysis was performed away from CSIRO, custom software was written in C. This enabled regions of the images to be manipulated in a more complex fashion. One of the difficulties in reproducing the AIS software values was the unknown scaling given to the above equation. The AIS gives a range of only 4000, when \(2^{16} = 65536\) are available. Hence the following scaling was introduced.

The above equation (Eq. 5.1) for \(p_{\text{size}} = 25\), has a maximum of \(p_{\text{size}}\text{max}_{25} = 2.5\), when QL is equal to its maximum value of \(2^{16} = 65536\). For \(p_{\text{size}} = 50\), the maximum \(p_{\text{size}}\text{max}_{50} = 10\). The minimum values are 0.00025 and 0.0010 for \(p_{\text{size}} = 25\) and \(p_{\text{size}} = 50\) respectively. Hence this value must be subtracted from the maximum before finding appropriate scaling factor (scpsl).

$$\text{scpsl} = \left(\frac{4000}{p_{\text{size}}\text{max} - p_{\text{size}}\text{min}}\right) \times (\text{psl} - p_{\text{size}}\text{min})$$  \hspace{1cm} (5.2)
CHAPTER 5. EXPERIMENTAL PRELIMINARIES

Figure 5.3: Artifact is just visible on the 25 µm scan as the faint vertical lines in the x-ray image and shown likewise in the line profile plot, which is the average of the columns.

This results in a scaling factor of 1600.02 for $p_{size} = 25$ and 400.04 for $p_{size} = 50$

5.1.3 Scanner resolution

Since resolution was important, it was thought that the 25 micron setting on the scanner would be preferred. However, this setting was found to suffer from an artifact that may have presented problems in quantitative analysis, see Fig. 5.3. Therefore, initially 50 micron scans were performed, which had the added bonus of being performed faster and with a smaller file size of 40 MB instead of 160 MB.

Unfortunately this setting often caused the system to lockup which could only be remedied by shutting down and re-initializing it again, which was a 20 minute process. Furthermore it was also determined that some scans with this setting did not
contain enough data points around the phase data peaks for accurate phase contrast measurements, hence the experimental work was repeated where necessary at the 25 micron setting. Care was taken to orientate objects at 90 degrees to the scanning direction so that the effect of the artifact could be minimized.

5.1.4 Characteristic curve

The characteristic curve of the system for a given tube potential (kVp) was determined by setting the tube current and varying the time of exposure and measuring the psl output. X-ray exposure is the product of the tube current and the time of exposure and is expressed in mAs. Five regions of pixels were chosen at various positions around the image and their values averaged to produce the table as shown in Table 5.1, and plotted for a tube potential of 30 kVp in Fig. 5.4. As can be seen from the graph, the system has a linear region between psl values ranging from 500 to 3700 and hence was

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the preferred range for experiments. Other kVp settings had a similar characteristic curve.

5.1.5 Image reproducibility

In order to measure quantities such as scatter and phase contrast accurately, the reproducibility of the imaging system needs to be considered. Variabilities between successive images include x-ray tube flux instability, shutter time inaccuracy for exposures, and scanner image plate reading differences. The simplest method is to take repeated images of the same object at the same settings and measure the brightness levels at several locations within the image. An ion chamber was used to check the
flux rate.

A test was performed for a 60 kVp tube voltage, 250 µA current with exposure time of 200 s at both 25 and 50 micron scan settings. Lead apertures were used to prevent unwanted scatter from objects inside the enclosure and the enclosure itself. One was placed near the source (at 2.3 cm), 8 mm in diameter and a second one, 10 cm in diameter, placed 74 cm from the source to further collimate the primary beam before entering 16 cm of perspex (poly-methyl methacrylate, PMMA). To filter out the low energy x-rays, 3.3 mm thickness of Aluminium which is typical clinical practice, was placed near the source.

A Radcal radiation monitor (model 1515), was positioned to measure the primary beam without obscuring the image formation by placing it just outside the second Pb aperture (see Fig. 5.5) which also prevents backscatter. A small diameter Pb disc was placed on the entrance side of the perspex to measure the amount of scattered radiation \( (S) \), whilst regions outside the disc are used to measure primary plus scattered radiation \( (S+P) \). An air gap of 10 cm was between the exit surface of the perspex and the image plate. The images plates had a physical size of 200 mm × 250 mm and were scanned with a sensitivity of \( s=4000 \), at \( p_{size}=50 \) and 25 µm resolution, and a graduation of 65536 = \( 2^{16} \). Five regions consisting of 100 × 100 psl values were chosen, four of which were outside the shadow of the lead disc and one inside as shown in Fig. 5.6. The results are shown in Table 5.2. A plot of these measurements is shown in Fig. 5.7, which show good stability over both the 50 and 25 micron settings, within the error bars. Note that the brightness levels differ between these settings due to the psl conversion formula. The ion chamber values were only used as a rough guide and the values are shown in the second part of the figure.
Figure 5.5: Schematic of image formation apparatus.

Figure 5.6: Measurement regions of the image
Table 5.2: Ion chamber primary flux readings plus psl primary plus scatter, and scatter values for 6 images which are the mean values of the regions. Error is calculated via the standard deviation of the region. Missing values are due to human error. Images 1-6 are recorded at \( p_{\text{size}} = 50 \mu m \), images 7-12 are recorded at \( p_{\text{size}} = 25 \mu m \).

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Figure 5.7: Graph of repeated images at 50 and 25 micron scanner settings
5.2 Test objects

One of the objectives of the thesis was to find a suitable object that showed good phase contrast that changed measurably with filters. Ideally the test object should be purely a phase object without any absorption, otherwise absorption contrast must be taken into account as well. Various objects were tested including edges, step wedges and hollow and solid fibres. The object found to be best suited was a hollow dialysis fibre (Cuprophan) made from cellulose ([C$_6$H$_{10}$O$_6$]$_n$) with an inner diameter of 200 $\mu$m and a wall thickness of 8 $\mu$m. Other objects are mentioned for interest and completeness.

5.2.1 Step wedge

Initial step wedges were made from overhead transparency, polyester type 1 (PET [C$_{10}$H$_8$O$_4$]$_{n=60-120}$) see Fig. 5.8, which is a low atomic number composition material, approximately 100 $\mu$m thick. This generated good phase contrast as can be seen in Fig. 5.9, even when used in conjunction with an Al filter, but was found to depend on the type of cut and horizontal alignment to the beam. Not only was it difficult to keep all edges aligned which may account for the staircase type pattern in the line profile, between some of the steps, but analysis using AIS$^TM$ software for profiles was limited.
to to either horizontal or vertical, but no other angle to allow for any misalignment. Thus a small error in alignment to the horizontal resulted in a large change to the computed phase contrast value.

Difficulties with the polyester type step wedges, led to trials from step wedges made from perspex or polymethylmethacrylate (PMMA $[C_5O_2H_8]_n$) which is another low atomic material with the ability to be easily machined. The first perspex step wedge was mill cut from a single block as shown in Fig. 5.10, with increasing thicknesses since the optimum thickness for phase contrast was unknown. An image containing the raw QL, psl corrected and line profile of this step wedge can be seen in Fig. 5.11. The image can be seen to be superior to the PET step wedge with better alignment of the edges. The largest phase peaks can be seen on the first and second steps from

![Figure 5.9: X-ray image of PET step wedge at 60 kVp, with aluminium filter.](image-url)
the air interface. This is due in part to the quality of the edge, as the milling process sometimes rounds the edge of the profile in the perspex.

5.2.2 Phase contrast variation with distance

With this test object, the distance from the source to the object, $r_s$, was varied from 5 to 50 cm. An empirical definition for the index of phase contrast minus the absorption contrast was calculated as

$$pc = \left( \frac{\text{max} - \text{min}}{\text{max} + \text{min}} \right)_{\text{peak}} - \left( \frac{\text{high} - \text{low}}{\text{high} + \text{low}} \right)_{\text{step}}$$  \hspace{1cm} (5.3)

A plot of this result can be seen in Fig. 5.12, where phase contrast is plotted against source to object distance for three of the steps. It can be seen that no conclusion may be
Figure 5.11: Perspex step wedge image with raw QI and psl correction and line profile. Air interface with the first step is on the right side. 

...easily drawn. Possible reasons for this are the changing angle of transmission that the steps present to the beam as \( r_s \) changes due to the fact that the solid angle subtended from the edge to the point source changes. This changes the transmission distance through the steps, which changes the attenuation and consequently the absorption contrast. Pogany et al. (1997) [65] showed that phase and absorption contrast have a complex relationship with distance from the source which is demonstrated in this experiment, where each step has a different profile and its phase contrast has a different relationship with distance from the source. This may further be complicated by the changing subtended area of each step, for averaging purposes, including more local non-uniformities which further affect the measurements. The next experiment was performed by keeping the distance between the source and the object fixed, and changing the filter position.
5.2.3 Effect of filter position

The effect of filter position was explored using the perspex step wedge and filters of aluminium and PMMA, with thicknesses 2 mm and 18.6 mm respectively. The step wedge was kept at a constant position of 25 cm from the source, using 30 kVp and 100 $\mu$A, and the image plate at 200 cm, while the filter was positioned both before and after the step wedge at 2, 20, 50, 100, 150, 198 cm. Line profiles from the AIS software can be seen in Fig. 5.14 for the aluminium filter (2mm) and Fig. 5.15 for the perspex filter (18.64 mm).

The line profiles with the aluminium filter can be seen to be increasing in brightness level as the filter is moved away from the source towards the detector. The one exception is the filter position at 198 cm which is almost touching the detector. A similar trend occurs when a PMMA filter is used, except that the 198 cm position has the brightest profile. This increase in brightness may be attributable to the order with
Figure 5.13: X-ray images of a step wedge various filter distances as measured from the source.

which the image plates were scanned, particularly if they were not erased sufficiently. For the case of the Al filter, successive images were taken at larger $r_s$ distances, so that if there were some residue left from incompletely erased plates then this might show as an increase in brightness. However, for the perspex filter case, the order of images was reversed, taken with successive decreasing $r_s$ distances, and the trend is still visible, except for the 198 cm distance for which the brightness trends are reversed for the two filters. This indicates that the effect is due to something other than image plate erasure effects such as scatter from the filter, enclosure or air.
Figure 5.14: Line profiles through PMMA step wedge x-ray image with differing filter (Al) positions. Note how the brightness of the profile increases with increasing filter distance position, except for the last position (198 cm) which is less bright than the 100 cm position.

5.2.4 Finer PMMA step wedge

Due to problems with the first PMMA step wedge, i.e being roughly cut and uneven steps, a second was made with more care and smaller step sizes. A photograph of this can be seen in Fig. 5.16 and Fig. 5.17. An x-ray image of this can be seen in Fig. 5.18 and it has a similar line profile to the PET step wedge. Even though the edges are much straighter than the PET step wedge, the phase contrast magnitude is much the same.

5.2.5 Other edges

Test objects with edges from different materials were tried, such as polycarbonate, cellophane, polyimide, lexan and teflon. Some materials had a naturally ‘sharp’ edge, while lexan for example had such a poor edge that it an attempt was made to polish it.
Figure 5.15: Line profiles through PMMA stepwedge x-ray image with differing filter positions (PMMA filter). Note how the brightness of the profile increases with increasing filter distance position, but particularly for the last position in opposite manner to the aluminium filter.

Figure 5.16: Second PMMA test object, with smaller and even steps
Figure 5.17: Second PMMA test object showing a better view of the step size

Figure 5.18: X-ray image of finer step PMMA wedge (on the left) together with PET step wedge (on the right)
These objects were attached to the PMMA step wedge for convenience and comparison, and imaged under the same conditions i.e. same kVp, μA, position but varying time exposures (see Fig. 5.19). The line profiles for these materials may be seen in Fig. 5.20. The cellophane and polycarbonate have good phase contrast compared to the PMMA step wedge, although they also have more absorption. The teflon, polyimide and lexan have relatively poorer phase contrast. The lexan despite polishing seems to be worse off than the unpolished sample. It may be that the edges were rounded rather than sharpened.

Figure 5.19: X-ray images of a step wedge together with edges made from materials: cellophane, polycarbonate, teflon, polyimide, lexan (unpolished) and lexan (polished).

The converse of an edge or step wedge is a grooved object. Since the first few steps in a wedge are very thin, there is the possibility of breakage or splitting while
machining. By cutting into a thicker material the edges are likely to maintain their integrity. The first one was made by cutting rectangular channels in a 5 mm thick piece of PMMA, of differing depths as shown in Fig. 5.21 and Fig. 5.22. A rather unexpected result from imaging this test object was the uneven distribution of the phase peaks across a gap edge as seen in Fig. 5.23. The phase peak on the left hand side of the groove was rarely the same as the phase peak on the right hand side edge, which may mean some anisotropy of the source as the same phenomena was noted when the object was rotated 180° (see Fig. 5.24). Furthermore tilting of the object from -2° to 2° also has little effect. It can be observed that the left hand side edge on each or the gaps/grooves, generally has a positive phase peak, while the right hand side

Figure 5.20: X-ray images of a step wedge together with edges made from materials: cellophane, polycarbonate, teflon, polyimide, lexan (unpolished) and lexan (polished).
each generally has a negative phase peak. If this were due to the physical condition of the edge, then upon rotating $180^\circ$, one would expect the peaks to reverse. The fact that they stay nearly the same, when a line profile is taken through the same region of the image in each case gives reason to believe that it must be a property of the x-ray beam. Although the spatial dimensions of the source are supposed to be smaller in the vertical direction ($\approx 4 \, \mu m$) and larger in the horizontal direction ($\approx 10 \, \mu m$), the shape and distribution are not known. It may be elliptically shaped for example with the semi-major axis inclined an an angle to the horizontal.
As a means of determining the best direction for phase contrast, a circularly grooved object was constructed. A photograph of this object can be seen in Fig. 5.25. By taking line profiles across the gap in a radial fashion, the phase contrast magnitude is dependent upon direction. An example is shown in Fig. 5.26 with the corresponding line profiles in Fig. 5.27.

As the angle of the line profile is increased from $0^\circ$, the positive peaks seen both edges revert to a single peak on the inside edge until $150^\circ$ and $180^\circ$ where they return again. From $210^\circ$-$300^\circ$, the positive peak only occurs on the outside edge, until $300^\circ$ and $360^\circ$ where both peaks can be seen again. The $0^\circ$ direction corresponds to the top of the image which means that the strongest phase contrast peaks correspond to the horizontal direction, which is also confirmed from the Au test object. However, the distribution of the source is still unknown.

Figure 5.23: Line profile through rectangular groove x-ray image. Note that the left phase peak is greater than the right on most grooves

Although these test objects gave reasonable phase contrast, they were not
Figure 5.24: X-ray image and line profile through rectangular groove x-ray image first one way then rotated 180°. Parameters 30 kVp, 100μA, 45 s, $r_s=28$ cm, $r_s + r_d=200$ cm
An associated problem with an edge is the repeatability of positioning it within the beam which becomes difficult with any change of $r_s$ distance as the height of the edge in the beam becomes another parameter.

A cylindrical object by comparison does not suffer from this problem as it has rotational symmetry and presents the same cross section regardless of vertical height.
Figure 5.27: Section of x-ray image through circular groove test object with radial line profiles at various angles. Profiles shown are averaged over 50 line profiles in close proximity. At 0° both edges give positive peaks, while for angles between 30° and 120° a positive peak is seen only on the inside edge while a negative one is seen on the outside edge. At 150° and 180°, positive peaks emerge on both edges, while from 210° to 300°, the positive peak occurs on the outside edge.

in the x-ray beam. It is therefore direction independent along the axis of symmetry. A selection of different fibres such as hairs, nylon fishing line and a feather are shown in Fig. 5.28. While the hairs and nylon fibre are clearly visible, the detail in the feather is most striking, and this gave the idea of a hollow fibre. The next section shows the results of imaging optical fibres, another nylon fibre and a hollow dialysis fibre.
5.2.6 Fibres

A number of fibres were tested, including two types of optical fibres, a solid nylon fibre, a hollow dialysis fibre, and a metallic copper fibre as shown in Fig. 5.29. As can be seen, the copper fibre has only absorption contrast, the optical fibre and nylon fibre have some phase contrast together with absorption contrast, but the dialysis fibre shows strong phase contrast with minimal absorption. Clearly this is the best phase object.

5.2.7 Dialysis fibres

Dialysis fibres are used for haemodialysis where they transport fluids by diffusion of solutes and ultrafiltration of fluid across a semi-permeable membrane. They are hollow
tubules made from low atomic number elements and come in a range of diameters and thicknesses. Importantly they present a symmetrical cross section to the beam, and are clean since sterile and do not require polishing as in the case of edges.

Different types of dialysis fibres were imaged with a region of interest shown in Fig. 5.31, where the fibres can just be seen.

An average of 100 lines in Fig. 5.32, shows the line profile for each fibre. The phase contrast was calculated for each fibre via the equation (Eq. 5.4), where absorption has been ignored and is shown in Table 5.3.

\[
pc = \left( \frac{\text{max} - \text{min}}{\text{max} + \text{min}} \right)_{\text{peak}}
\]  

(5.4)

The last fibre shows the greatest phase contrast and hence was used for subsequent

Figure 5.29: X-ray image of various fibres with line profile. Note the good phase contrast with little absorption of the Cuprophan fibre
### Capillary Membranes for Haemodialysis

<table>
<thead>
<tr>
<th>Application</th>
<th>Membrane</th>
<th>Basic Polymer</th>
<th>Yel thickness (µm)</th>
<th>Inner Diameter (µm)</th>
<th>Hydrated permeability in relation to blood pressure (with/without)</th>
<th>Hydrated permeability with water (dehydration)</th>
<th>Sodium-Carbonate</th>
<th>Abnormal</th>
<th>Mean pore diameter (µm)</th>
<th>Cell structure</th>
<th>Shear test</th>
<th>Possible specification model</th>
</tr>
</thead>
<tbody>
<tr>
<td>low flux</td>
<td>CUROPHAN® RC55</td>
<td>regenerated cellulose</td>
<td>6</td>
<td>200</td>
<td>5.4</td>
<td>no criteria</td>
<td>no criteria</td>
<td>4.5</td>
<td>9</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>low flux</td>
<td>HEMOPHAN® MC55</td>
<td>DEAD-synthetically modified cellulose</td>
<td>6</td>
<td>200</td>
<td>5.4</td>
<td>no criteria</td>
<td>no criteria</td>
<td>4.5</td>
<td>9</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>low flux</td>
<td>SMC® BXX</td>
<td>Bio-synthetically modified cellulose</td>
<td>9</td>
<td>200</td>
<td>6.9</td>
<td>no criteria</td>
<td>no criteria</td>
<td>4.4</td>
<td>10</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>low flux plus</td>
<td>SYNPHAM® LP400</td>
<td>poly-Ethylsulfone</td>
<td>35</td>
<td>200</td>
<td>12</td>
<td>no criteria</td>
<td>no criteria</td>
<td>5.7</td>
<td>20</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>mid-flux</td>
<td>SYNPHAM® HF200</td>
<td></td>
<td>35</td>
<td>200</td>
<td>15</td>
<td>0.05</td>
<td>0.00</td>
<td>64.5</td>
<td>25</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>high flux</td>
<td>SYNPHAM® HF500</td>
<td></td>
<td>30</td>
<td>200</td>
<td>37</td>
<td>0.5</td>
<td>0.005</td>
<td>84.0</td>
<td>50</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>super high flux</td>
<td>SYNPHAM® HF800T</td>
<td></td>
<td>30</td>
<td>200</td>
<td>38</td>
<td>0.03</td>
<td>0.01</td>
<td>84.0</td>
<td>50</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

---

*mmHg = 1.333 kPa*  
*P = 0.45*  
*P = 0.45*  
*PEET = Performance Enhancing Technology*  
*Y determined by double test method of a molecule having 97% water in each method will yield similar result*  
*All products available as non sterile, direct bundles, according to customer agreed specification, ready to use.*
Figure 5.31: A magnified portion of the x-ray image of various types of dialysis fibres.

Figure 5.32: 100 averaged line profile showing phase contrast of the fibres.
Table 5.3: Table of calculated phase contrast values for different dialysis fibres as shown in Fig. 5.32.

<table>
<thead>
<tr>
<th>fibre</th>
<th>phase contrast</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.1036</td>
</tr>
<tr>
<td>2</td>
<td>0.1095</td>
</tr>
<tr>
<td>3</td>
<td>0.0907</td>
</tr>
<tr>
<td>4</td>
<td>0.0759</td>
</tr>
<tr>
<td>5</td>
<td>0.0848</td>
</tr>
<tr>
<td>6</td>
<td>0.1948</td>
</tr>
</tbody>
</table>

Figure 5.33: Cuprophan fibre stretched across custom made holder. The sticky material (Blu tak) on the edge of the frame near the fibre enables a mirror to be attached for positioning in the x-ray beam as indicated by the red laser beam.

experiments. This fibre was a type Cuprophan RC55 from Membrana and is shown in Fig. 5.33. It is made from regenerated cellulose with a wall thickness of 8 \( \mu \text{m} \) and an inner diameter of 200 \( \mu \text{m} \). An optical microscope image of it is shown in Fig. 5.34, where there is a strong reflection of the light source that should not be confused with the edge.

One problem associated with phase contrast measurement is the noise. A single line profile has so much noise that it swamps the signal, therefore it is common practice to average over many line profiles which reduces the noise by a factor \( 1/\sqrt{N} \), where \( N \) is the number of averaged lines, assuming the noise is random and normally distributed.
The amount of noise compared to signal can be seen in the surface plot Fig. 5.35. It is impossible to see any discernable edge, however in the image just below two faint edges can just be seen. This illustrates the necessity of averaging enough to increase the signal to noise ratio (SNR), but too many can decrease the measurement due to bending or misalignment of the fibre. In Fig. 5.36, individual profiles can be seen for the first three rows together with 100 averaged such line profiles. It can be seen that the noise is very high but that it decreases with signal averaging. In Fig. 5.37 the variation of phase contrast with the number, $N$, of averaged profiles is shown. If the fibre were perfectly uniform, straight and perfectly horizontally aligned, phase contrast would be constant. Since it neither of these, phase contrast is function of the averaging number.
5.3 Fibre straightening

This previous section shows the difficulty of obtaining a reliable phase contrast index that is not subject to limitations of averaging. Restricting an ROI to a uniform and straight section of the fibre can overcome some imperfections, however perfect alignment is extremely difficult. An alternative is to straighten the fibre via software. It can be seen for example in Fig. 5.38, that a straight edge against the right fibre edge shows that the fibre is not vertical. A program was written to translate the rows of the image such that it matches some criterion. In this case the cross correlation coefficient. Individual rows are tested against the averaged line profile for correlation, and an index is returned for the maximum correlation. It is not necessary to test every value in the row but some limited range around the average peak positions. This was chosen to 20
Figure 5.36: Individual line profiles through the selected region plus a 100 averaged line profile shown in red.

points, which more than adequately covers the region of the phase contrast peaks.

Originally the line profile was kept intact, assuming the width of the fibre would remain constant, so that each edge was moved by the same amount. This resulted in an improved image, but a better procedure was to cut the image vertically in half between the edges and treat them separately. This resulted in the straightened image Fig. 5.39.

As can be seen this results in a greatly improved alignment, and furthermore if phase contrast is now calculated as a function of line averaging number the left edge shows dramatic improvement and converges quickly to around 0.11 after about 100 lines, see Figure 5.40. The right edge decreases from about 0.1 to 0.08, but again
Figure 5.37: Phase contrast as a function of averaging number.

<table>
<thead>
<tr>
<th>edge</th>
<th>raw</th>
<th>psl</th>
<th>straightened</th>
<th>double straightened</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.015768</td>
<td>0.13912</td>
<td>0.14085</td>
<td>0.1403</td>
</tr>
<tr>
<td>2</td>
<td>0.0062173</td>
<td>0.054668</td>
<td>0.1066</td>
<td>0.1428</td>
</tr>
</tbody>
</table>

Table 5.4: Table of calculated phase contrast values for raw and psl images.

shows fast convergence.

An improvement for the right edge is to correlate to one particular line say the last or the first. Finding the average tends to spread the edge further. Thus keeping all correlations to one edge shows marked improvement. Double straightening the image improved the right edge by another 25%, but $4	imes$ was shown to be sufficient to bring both edges to a convergent result as shown by Figures 5.42, 5.43, 5.44, 5.45, 5.46 and 5.47.
5.4 Scatter measurements

Previous work [3] examined the measurement of scattered radiation in fluoroscopic and radiographic situations. This involved the placing a small lead disc in the beam to block the primary radiation, so that measurements in its shadow give an estimate of the magnitude of scattered radiation. This technique was used as early as 1921 by Wilsey [133], and makes no distinction between coherent and incoherent contributions.
Figure 5.39: Fibre section showing edges now vertical.

To overcome the error involved by the introduction of the Pb disc, a commonly used technique is to use a range of lead discs sizes and to back extrapolate the measurements to zero size (see Boone 1986 [163]). As was discussed, a question arose regarding the measurements of scatter by small disc sizes (< 1 cm) which may have been influenced by off-focal radiation in the x-ray tube and/or veiling glare effects in the detector. The system used for these measurements was a Toshiba mobile fluoroscopic x-ray apparatus (SXT - 6 - 11) with a nominal focal spot size of 0.5 mm, and an image intensifier detector system. The opportunity naturally arose to answer this question using the Feinfocus
source and detection system used for this study. Designed specifically for spatial coherence, the microfocus source has very highly focussed electron beam, thereby reducing off focal radiation, and the image plate detection system, described more fully in the next section, is likely to have minimal veiling glare compared to an image intensifier system.

In a similar method to the reproducibility measurements, Pb discs with varying diameters are used to measure scattered radiation as shown in Table 5.5. However the reference regions outside the disc now change as the disc size becomes larger and are no longer particularly indicative. The first two columns are graphed in Fig. 5.48 together with the predictions of the model described in chapter 3, scaled to the scatter measurements of the 1 cm and 0.3 cm discs, since the model predicts relative rather...
Figure 5.41: Phase contrast as a function of averaging number after fibre straightening.

Figure 5.42: Edge straightening program
Figure 5.43: Un-straightened averaged line profile

Figure 5.44: Once straightened averaged line profile

Figure 5.45: Twice straightened averaged line profile
Figure 5.46: Four times straightened averaged line profile

Figure 5.47: Phase contrast as a function of iteration number
than absolute values. These two values were chosen as they were close in physical size to the increments used in calculating the model. The 1 cm disc was ultimately chosen as the standard to scale the model predictions as it was less likely to suffer from off focal radiation and glare effects.

Table 5.5: Scatter measurements using lead discs with reference regions

<table>
<thead>
<tr>
<th>Disc diameter (mm)</th>
<th>disc region</th>
<th>region 1</th>
<th>region 2</th>
<th>region 3</th>
<th>outside region</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.77</td>
<td>1930</td>
<td>3387</td>
<td>2671</td>
<td>1937</td>
<td>1925</td>
</tr>
<tr>
<td>2.15</td>
<td>1923</td>
<td>3415</td>
<td>2699</td>
<td>1914</td>
<td>1898</td>
</tr>
<tr>
<td>2.44</td>
<td>1942</td>
<td>3415</td>
<td>2731</td>
<td>1933</td>
<td>1894</td>
</tr>
<tr>
<td>3</td>
<td>1879</td>
<td>3310</td>
<td>2614</td>
<td>1929</td>
<td>1915</td>
</tr>
<tr>
<td>3.49</td>
<td>1933</td>
<td>3440</td>
<td>2726</td>
<td>1910</td>
<td>1889</td>
</tr>
<tr>
<td>3.99</td>
<td>1933</td>
<td>3445</td>
<td>2706</td>
<td>1907</td>
<td>1903</td>
</tr>
<tr>
<td>4.92</td>
<td>1832</td>
<td>3260</td>
<td>2588</td>
<td>1910</td>
<td>1885</td>
</tr>
<tr>
<td>6.11</td>
<td>1856</td>
<td>3305</td>
<td>2624</td>
<td>1909</td>
<td>1884</td>
</tr>
<tr>
<td>7.01</td>
<td>1865</td>
<td>3275</td>
<td>2619</td>
<td>1935</td>
<td>1897</td>
</tr>
<tr>
<td>10.23</td>
<td>1841</td>
<td>3325</td>
<td>2623</td>
<td>1882</td>
<td>1870</td>
</tr>
<tr>
<td>20.03</td>
<td>1758</td>
<td>3355</td>
<td>2654</td>
<td>1836</td>
<td>1764</td>
</tr>
<tr>
<td>42.31</td>
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<td>1561</td>
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<tr>
<td>74.08</td>
<td>1001</td>
<td>2460</td>
<td>2256</td>
<td>1383</td>
<td>1182</td>
</tr>
<tr>
<td>99.6</td>
<td>537</td>
<td>1940</td>
<td>1836</td>
<td>941</td>
<td>779</td>
</tr>
<tr>
<td>115.6</td>
<td>224</td>
<td>1610</td>
<td>1610</td>
<td>371</td>
<td></td>
</tr>
<tr>
<td>4.92</td>
<td>1883</td>
<td>3330</td>
<td>2642</td>
<td>1922</td>
<td>1899</td>
</tr>
<tr>
<td>2.44</td>
<td>1874</td>
<td>3320</td>
<td>2630</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The results show reasonable agreement between the model and experiment. Use of the micro-focus source reveals that at small disc sizes less than 1 cm, the measured scatter values follow the model more closely than measurements from the Toshiba system, which were possibly contaminated by off focal radiation or detector veiling glare effects. See Fig. 5.49 which shows measurements made with the fluoroscopic system for comparison. This was the original purpose of the model, as linear extrapolation of the disc sizes is likely to overestimate the amount of scatter. Thus given a scatter measurement from a 1 cm Pb disc for scaling, the model should give a good estimate of the disc free scatter value without the need for further measurements and using linear extrapolation. In a clinical setting this would reduce patient dose. For the purposes
Figure 5.48: X-ray scatter measurements using a microfocus source, versus Pb disc diameter together model calculations.

of this thesis, it may also be used to estimate the amount of incoherent scatter from either the filter, object or both, and therefore it was considered worthwhile to refine the model further.

### 5.4.1 Scatter variation with air gap

It is well known that the air gap between the object and the detector has an important influence on the amount of detected scatter. Ideally the model should reflect this since phase contrast requires a relatively large air gap for interference effects to be visible, and knowing the extent of incoherent scatter reaching the detector would be useful.

Therefore exploring this effect, experiments were performed for three different distances of 5, 10 and 15 cm and the results are shown in Fig. 5.50. The calculations
CHAPTER 5. EXPERIMENTAL PRELIMINARIES

Figure 5.49: Experimental data obtained with mobile Toshiba fluoroscopic machine with 0.5 mm nominal source size.

from the model were scaled to the 1 cm diameter disc of the 5 cm air gap which has the greatest amount of scatter and the same factor was used for the 10 and 15 cm cases. As can be seen the fit to the 5 cm data is very good, but systematically over estimates the measured values for the 10 and 15 cm cases by about 12%, but nonetheless still follows the general trend. Although not quantitatively accurate for these greater air gaps, it is nonetheless qualitatively correct and still useful to have an upper limit for scatter magnitudes for larger air gaps.

A plot of variation scatter (S) and primary plus scatter (P+S) with air gap for the 1 cm diameter disc is shown in Fig. 5.51. As can be seen, both S and S+P fall away with increasing distance and S is reduced significantly for large air gaps greater than 50 cm. By subtracting the scatter values for the scatter plus primary values, the primary beam variation can be calculated. By taking natural logarithms of the intensity and
the air gap values, it can be shown that the dominant variation is due to the inverse square law, and that the attenuation in the air is negligible.

A relationship for the variation by the inverse square law and the extra attenuation by the air can be written mathematically as

$$I = \frac{I_0}{(s + a + \tau)^2} e^{-\mu_a(s+a)-\mu_p\tau}$$  \hspace{1cm} (5.5)$$

where $I_0$ is incident intensity, $\mu_a$ and $\mu_p$ are the linear absorption coefficient of air and perspex respectively, $s$ is the distance from the source to the object, $a$ is the air gap and $\tau$ is the thickness of perspex. Increasing the air gap causes only the variable $a$ to
change, and by taking natural logarithms this becomes

\[ \ln I = \frac{\ln(I_0) - \mu_a s - \mu_p \tau - \mu_a a - 2 \ln(s + a + \tau)}{K} \]  
\[ = K - \mu_a a - 2 \ln(s + a + \tau) \]  

(5.6)

where \( K = \ln(I_0) - \mu_a s - \mu_p \tau \) is a constant. If the attenuation through the air were considered negligible (\( \mu_a a \approx \mu_a s \approx 0 \)), then this equation would be

\[ \ln I = K - 2 \ln(s + a + \tau) \]  

(5.7)

Therefore a plot of \( \ln I \) and \( \ln(s + a + \tau) \) should produce a graph with a slope equal to -2 and this can be seen in Fig. 5.52, where the first data point has been ignored. Since the plot has very few values it is not a strong conclusion, but it seems to indicate that the inverse square law is the most likely mechanism for the primary beam intensity to
fall off with air gap. Hence in the modelling process, the attenuation due to air was neglected.

![Logarithmic plot of total distance and intensity showing a gradient of -2. The first point has been ignored.](image)

Figure 5.52: Logarithmic plot of total distance and intensity showing a gradient of -2. The first point has been ignored.

Now the primary intensity can be plotted against the total distance as shown in Fig. 5.53. The equation for the intensity is

\[
I = \frac{e^{15.586}}{(s + \tau + a)^{2.02}}
\]  

(5.8)

where \(I_0 = e^{15.586}\) and it can be seen that it fits the data very well.

### 5.4.2 Scatter variation with thickness

As the thickness of the object increases, there is an increased likelihood of multiple scatter. In this case the asymmetry associated with individual events of Compton scattering is likely to be evened out and the predictions of the model are likely to
Figure 5.53: Primary radiation intensity versus total distance together with an inverse square relationship.

become better. A plot is shown in Fig. 5.54 of two different thicknesses of perspex and the resulting scatter measurements for various disc sizes. The first thickness of perspex was 8 cm, with a source to object distance of 80 cm, and a 10 cm air gap to the image plate. The beam was filtered with 3.3 mm Al and the beam was collimated near the source by a small rectangular aperture, and another 10 cm diameter circular aperture at the perspex to limit the beam to the perspex and not to the sides or floor of the enclosure. More perspex sheets were added to the source side to increase the thickness to 14 cm, keeping the air gap and source to detector distance the same. This changed the source to perspex distance to 74 cm, and since the discs are mounted on the first perspex sheet, this changes the angle of shadow of the disc slightly but this is preferable to changing the other parameters.

The model with separate scaling factors is reasonably good, however with the same scaling factor it overestimates the amount of scatter going from the 8 cm case to the 14 cm case, by nearly 40% at the zero disc size. This may be due to the lack of
attenuation in the model. To include attenuation requires calculating the path of the primary beam through the object to the scatter site, and the path of the scattered signal to the detector site. By geometry the path of the primary beam, \( l \), see Fig. 4.9, through the perspex is found to be

\[
l = (t - z) \sqrt{\frac{r^2}{(t - z + s)^2} + 1}
\]  

The corresponding path length of the scattered beam through the perspex, \( L \), is found to be

\[
L = \left(\frac{z}{z + a}\right) \sqrt{(z + a)^2 + r^2 + q^2 - 2rq \cos(\psi - \phi)}
\]
This means that the scatter function \( h(q, \psi) \) is now modified to

\[
h(q, \psi) = \int_{r} \int_{\phi} \int_{z} \frac{r(z + a)e^{-\mu(L+l)}}{[r^2 + q^2 - 2rq \cos(\psi - \phi) + (z + a)^2]^{3/2}} dr d\phi dz
\]

(5.11)

Unfortunately, this integral cannot be evaluated analytically as before and requires numerical integration over the three integrals which increases the calculation time dramatically. Since the linear attenuation coefficient \( \mu(\varepsilon) \) is a function of energy, this triple integral must be performed for each component of the energy spectrum. This requires knowledge of the x-ray tube spectrum and the relative amounts of the intensity for each energy. A very rough method to measure the linear attenuation coefficient is to collimate the beam and measure the brightness with and without the object. This was done using a 1 mm diameter aperture, 15 cm of PMMA and a very large air gap of 185 cm which ensures very little scatter reaches the detector and only primary radiation is measured. Using the Beer-Lambert law,

\[
I = I_0 e^{-\mu t}
\]

where \( I \) and \( I_0 \) are the attenuated and incident intensity respectively, \( \mu \) is the linear attenuation coefficient and \( t \) is the thickness, the attenuation is given by

\[
\mu = \frac{\ln I_0 - \ln I}{t}
\]

This gives an estimate of \( \mu = 0.37 \), which is not a true reading but an average reading of the polychromatic spectrum. This is close to the value (0.3702) by Tsai and Cho (1976) [164] for a 27 keV monoenergetic beam.

At this point, without too much difficulty, the primary beam intensity may also be calculated. It is a simple variation of the primary beam attenuation of before, except simplified as it traverses the entire thickness of the object. The path length, \( l_p \), through the solid is found to be

\[
l_p = \sqrt{\left(\frac{qt}{s + t + a}\right)^2 + t^2}
\]

(5.12)

An example of simulated scatter with primary beam attenuation is shown in Figs. 5.55 and 5.56.
5.4.3 Scatter variation with filter position

The model may be used to test whether scatter is occurring from the filter that may affect phase contrast measurements. This is easiest to perform when the filter is PMMA rather than Aluminum, as the line profiles show a monotonic increase with filter position, particularly with the filter position at 198 cm, i.e. closest to the detector, whereas the Al case showed initially an increase, then a decrease for the last measurement see Fig. 5.14 and Fig. 5.15. The psl values extracted from the line profiles for each step are shown in Table 5.6. These are assumed to be composed of primary beam plus scattered radiation. Counting from the thickest part of the step wedge, the psl values from the 10th step which corresponds to the air, the primary field is assigned to the value for the largest air gap, i.e. least scatter. This corresponds
Figure 5.56: Simulated 2D image of lead (Pb) disc by photoelectric effect and scatter. Vertical and horizontal axis are both position (in data points)

to a filter position of 2 cm (air gap of 198 cm), i.e. P=2378. Subtracting this from the primary plus scatter values for the entire row gives a measure of the relative scatter.

To calculate the relative scatter from the model, the dimensional parameters are entered into the program for two sets of geometries. The filter was a 5 cm by 5 cm block of perspex. This was converted to an equivalent circular area and the radius deduced as 2.82 cm for the axial symmetry used in the program. The air gap and filter position varied together while the source to detector distance was kept constant. Parallel
Table 5.6: Psl measurements for each step at various filter positions (cm) (Air gap = 200 - filter position).

<table>
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<tr>
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<tr>
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<td>1918</td>
<td>1853</td>
<td>1800</td>
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and diverging beam geometries were both used, and all calculations were converted to normalized values including the experimental ones. The comparison is shown in Fig. 5.57. It can be seen that there is little difference between parallel and diverging beam geometries, but both underestimate the scatter occurring in the experiment. Adjusting the field size parameter to 50 cm radius proves a better fit of the model, however this does not match the physical dimensions of the filter. There is also an artifact near the end of this graph due to sensitivities to small values approaching zero.

It is possible that there may be extraneous scatter coming from the walls and floor of the enclosure which has a roughly a 50 cm radius with the center of the beam offset to about 30 cm from the floor. The surrounding air may also be influencing these measurements. An indication of this is shown in Fig. 5.58, where an Pb aperture was used to reduce the x-ray beam, to see if it affected the overall brightness of the image. A square aperture with dimensions 19 mm × 19 mm, was placed at a distance of 14 cm from the source, while the step wedge was placed at 25 cm. This limited the beam to an effective field size of 5 cm at the test object and excluded the beam from reaching the enclosure. A 2 mm, Al filter was positioned at 6 cm from the source. An interesting observation is that the use of an aperture affects the brightness of the line profile of
Figure 5.57: Comparison of experimental scatter values and model with diverging beam for PMMA filter.

Figure 5.58: Line profiles through a PMMA step wedge showing the effect of using an aperture.
Figure 5.59: Line profiles for an x-ray image of a fibre with various apertures showing the increase in brightness when no beam apertures are used.

the filtered profile more so than the unfiltered case.

A similar experiment using two collimators, and a larger area Al filter show that the predominant source of scatter is not from the filter. A circular aperture of 0.74 cm diameter was placed at a distance of 13.5 cm from the source, with a second 2 cm square aperture located at 48 cm from the source. The second aperture results in a projected area at the screen of 8.3 cm × 8.3 cm. This prevents the beam from scattering from the enclosure. The test object used in this case was a Cuprophan fibre and line profiles are shown in Fig. 5.59. It can be seen that the line profiles are much the same for either both apertures in place or just the 0.74 cm aperture which results in a projected diameter of 11 cm at the detector. However when both apertures are removed, the line profile shows a 5% jump in brightness. When an Al filter of larger dimension (10 cm diameter), was used in various positions in the beam, the psl values were found to be practically identical. See Fig. 5.60. Without extensive modelling of these effects it is difficult to determine the exact source of the scatter, but it does
lead to the conclusion that filters should be used as far from the detector as possible if collimators are not used. However, for the purpose of phase contrast, thin filters as are commonly used in clinical practice, while influencing the beam, are not causing phase contrast loss by the mechanism of scattering.

5.5 Summary

This chapter has outlined the basis of the image system from the source to the detector, and determined a method of analyzing the images. The model for incoherent scatter has been tested for air gap and thickness. In its simplest form it is useful as a rough guide to the relative amount of scatter in a given imaging set up, due to the ease of calculation. However for more accurate estimates, attenuation effects should be included to allow for the possibility of comparison between object and filter materials. This inclusion means

Figure 5.60: Line profiles for x-ray image of a fibre with larger area filter at various positions showing similar brightness levels and that scattering is not occurring from the filter.
that the integrals no longer simplify algebraically and therefore must be evaluated numerically which consequently increases the calculation time. Furthermore it requires knowledge of the x-ray tube spectrum, which necessitates another lengthy calculation. Although the scatter has been modelled as isotropic, it could be extended by inclusion of the Klein-Nishina equation to allow for a more realistic scatter distribution. This would require keeping track of all the angles from the object to the detector in a similar manner to Inanc 2002 [159]. A further step to include absorption and coherent scatter would make the model more general and allow for the possibility of calculating dose in an object or possible patient. This however was beyond the scope of the thesis, as the relative amounts of incoherent scatter influencing phase contrast measurements from small objects such as fibres is almost negligible.

The effect of filters from a scattering point of view was found to increase the overall brightness of an image, as the filter was systematically positioned nearer to the detector. Determining the cause of this was investigated, as whether it originated as scattering of the x-rays from the bulk material in the filter or background scatter around the filter from the enclosure or air. Using the simple model and various geometries it was found that scattering based on a ray optical model of scattering and the thickness of the 18.6 mm PMMA filter, was only significant when the filter was closer than 10 cm from the detector. This was considerably less by a factor of 8 than the deduced amounts of scatter made from experiments, indicating this was not the main mechanism. When apertures were used to restrict to the x-ray beam to the size of the detector, preventing contamination from sides of the operating enclosure, the brightness level was found to drop with all filter positions. This affected the protocol of obtaining phase contrast measurements to placing the filter closer to the source and far from the detector and/or collimating the beam to restrict background scatter.
Chapter 6

Experimental

This chapter discusses in detail the effect of four main imaging parameters on phase contrast with respect to the Cuprophan RC55 dialysis fibre chosen from chapter 5 (section 5.2.7) as the test object. These parameters are the tube current ($\mu$A), tube potential (kVp), beam filtration material, and the geometrical distances between the source to object ($r_s$) and object to detector ($r_d$). The tube potential and beam filtration affect the x-ray beam spectrum, whereas the tube current and the magnification factor ($r_s + r_d/r_s$) affect the imaging geometry and all showed significant effect on phase contrast measurement.

The tube current influences the source size and was investigated for source sizes from 4 to 50 $\mu$m while keeping the x-ray flux constant and measuring the phase contrast after straightening the fibre image by software described in chapter 5. Similarly, tube potential was investigated in 30 kVp increments from 30 to 150 kVp, while maintaining the source size at 4 $\mu$m. In the case of the filter experiments, materials such as Al, Au and PMMA of various thicknesses were inserted into the beam close to the source and except where stated, with collimation. Geometrical magnification factors were investigated using source to object distances ($r_s$) from 0.5 to 193 cm, while the object to detector distance $r_d$ changed correspondingly as the total distance between source
to detector \((r_s + r_d)\) was kept at a constant 200 cm. Some other factors investigated were the grain size of the aluminium filters, which was found to have little influence, and the noise introduced by filters which showed no appreciable difference from the unfiltered case. Similarly it was found that the filter surface, and orientation also had little effect indicating that the phase reduction is a bulk material effect. The technique of blank field subtraction which is often used to eliminate image non-uniformities, was used to try and improve phase contrast measurements but was found to have no effect, possibly because the fibre region was so small.

To investigate the beam spectra from the tungsten target with the applied tube potential and effect of beam filters, it was initially simulated using XOP and Xcomp5r software programs. However since these showed significant difference in their predicted spectra the spectra was measured using a SiLi detector in conjunction with various filters.

### 6.1 Phase contrast variation with source size

Since phase contrast is dependent upon source size, this parameter was explored by altering the tube current. Systematically doubling the tube current and halving the exposure time, maintains a constant x-ray flux but increases the focal spot size via the target overheating protection mechanism of the tube. The source size relationship to the electron beam energy is shown in Fig. 6.1, provided by Feinfocus. To find the focal spot size, the tube potential (kVp) is multiplied by the tube current (\(\mu A\)) to obtain the energy in Watts. For example the settings at 30 kVp, 100 \(\mu A\) gives 3 W, and this corresponds to about a 4 \(\mu m\) spot size for the tungsten target.

A series of images with \(r_s=5.5\) cm and \(r_d=194.5\) cm, 25 \(\mu m\) resolution using three different image plates were taken at 30 kVp tube voltage, with varying tube currents as shown in Table 6.1.
Figure 6.1: Source size estimation from input power graph (Feinfocus)
Table 6.1: Source size data including image number, image plate number, tube voltage, tube current, time of exposure, approximate source size and brightness of image (psl)

<table>
<thead>
<tr>
<th>Image</th>
<th>Plate</th>
<th>Voltage (kVp)</th>
<th>Current (µA)</th>
<th>time(s)</th>
<th>size (µm)</th>
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Figure 6.2: X-ray images of a Cuprophan fibre for various focal spot sizes, at 30 kVp, r_s=5.5 cm, r_d=194.5 cm, and scanned at 25 µm resolution.
Figure 6.3: X-ray phase contrast variation with tube current, with approximate source sizes, at 30 kVp, $r_s=5.5$ cm, $r_d=194.5$ cm, and scanned at 25 µm resolution.

Representative images with associated line profiles are shown in Fig. 6.2 for source sizes from 6-50 µm. The difference between 4 and 6 µm is minor, while a dramatic difference can be seen for 25 µm in which the fringes appear to increase in number, thereby decreasing the visual acuity of the fibre, until for 50 µm the fringes are completely washed out and almost no phase contrast is visible. This is reflected in the phase contrast calculation for each condition as shown in Fig. 6.3, which shows phase contrast with increasing tube current. The corresponding source size dimensions are marked by arrows. It can be seen that after 400 µA which corresponds to about 12 µm, that the phase contrast reduces steeply, and that phase contrast strongly depends upon the geometrical factor of source size.
6.2 Phase contrast variation with tube potential

The tube voltage affects the energy x-ray spectrum emitted from the tungsten target. For optimal phase contrast, as shown in Section 6.1, the source must be focussed to its smallest spot. Focussing of the Feinfocus x-ray tube, as mentioned in Section 5.1.1, is achieved manually by acquiring an image of a gold mask test object (Fig. 5.1), determining how many line pairs are visible by inspection, then changing the focus settings and repeating the process until maximum visibility is achieved. Since this is a rather tedious process, only 30, 60, 90, 120 and 150 kVp tube potentials were focussed to investigate the effect on phase contrast.

Figure 6.4: X-ray images of Cuprophan RC55 fibre at 30 and 60 kVp, with rs=5.5 cm, rd+rs=2 m, all at 25 micron detector setting. The second and third 30 kVp images were acquired with a tube current of 200 µA, as the first 100 µA image was performed at the wrong rs value and the third image was overexposed. Note also that the first 60 kVp image is also overexposed.

Images of a fibre at these potentials can be seen in Fig. 6.4, and Fig. 6.5. These
Figure 6.5: X-ray images of Cuprophan RC55 fibre at 90, 120 and 150 kVp all at 25 micron detector setting, and $r_s=5.5$ cm, $r_d+r_s=2$ m.

show all image plates used with their various exposure times which was done to ensure that at least one of the images has the correct brightness level, although often all images were in the correct range. The source size is kept the same when the tube potential is changed as the tube current is adjusted to compensate automatically. Due to a mistake there is only one image at 30 kVp and 100 $\mu$A as the first image was performed at a different $r_s$ value and third was overexposed. Therefore phase contrast from two images using 200 $\mu$A are included into the graph shown in Fig. 6.6, as the values are fairly close (see section 6.1).

Since each voltage setting requires a different exposure time, the images vary somewhat in absolute brightness but as was shown in the previous chapter, this does
not affect the phase contrast index. This information including tube voltage, current, image plate number, exposure time, focal spot size, approximate psl brightness and calculated phase contrast with errors for left and right edges is shown in Table 6.2. The geometry was $r_s=5.5$ cm and $r_d=194.5$ cm, and all images were scanned at 25 $\mu$m resolution.

Each successive increase in voltage, shows a loss of acuity of the fibre and increased graininess. The variation of phase contrast index with tube voltage can be seen in Fig. 6.6, which shows a systematic decrease in phase contrast with increasing voltage. An exception is at 60 kVp which seems to show slightly less phase contrast than 90 kVp, but it is most likely that the tube was not properly focussed at 60 kVp. The best phase contrast occurs at 30 kVp. The errors have been calculated via Section 6.4.2.

Thus except for the inherent Be filtration of the tube, the variation of phase contrast
Table 6.2: Data including image number, image plate number, tube voltage (kVp), tube current (µA), time of exposure (s), approximate source size (µm), rough brightness of image (psl), phase contrast values (γ) for left and right edges and their associated errors

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<th>Plate</th>
<th>kVp</th>
<th>µA</th>
<th>time(s)</th>
<th>size (µm)</th>
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</table>

without added filtration decreases with increasing tube potential.

6.3 Phase contrast variation with source to object distance

The other geometrical factor investigated affecting phase contrast is the distance ratio between source to object, $r_s$, and object to detector, $r_d$. The total distance from source to detector was kept constant at $r_s + r_d = 200$ cm, hence the magnification varies as $200$ cm/$r_s$. The $r_s$ and $r_d$ distances were systematically varied and the results are tabulated in Table 6.3. The experiments were conducted with a tube voltage of 30 kVp and tube current 100 µA, which corresponds to a source size of about 4 µm, and the detector resolution setting was 25 µm.
CHAPTER 6. EXPERIMENTAL

Table 6.3: X-ray phase contrast values ($\gamma$) for images of a fibre with changing $r_s$ and $r_d$ values, at 30 kVp, and scanned at 25 $\mu$m resolution.

<table>
<thead>
<tr>
<th>$r_s$ (cm)</th>
<th>$r_d$ (cm)</th>
<th>mag.</th>
<th>$\gamma_{leftnoA}$</th>
<th>$\gamma_{rightnoA}$</th>
<th>error</th>
<th>$\gamma_{leftedge}$</th>
<th>$\gamma_{rightedge}$</th>
<th>error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>199.5</td>
<td>400</td>
<td>0.192</td>
<td>0.190</td>
<td>0.003</td>
<td>0.090</td>
<td>0.066</td>
<td>0.003</td>
</tr>
<tr>
<td>0.5</td>
<td>199.5</td>
<td>400</td>
<td>0.105</td>
<td>0.099</td>
<td>0.003</td>
<td>0.200</td>
<td>0.194</td>
<td>0.003</td>
</tr>
<tr>
<td>5.5</td>
<td>194.5</td>
<td>36.3</td>
<td>0.214</td>
<td>0.215</td>
<td>0.003</td>
<td>0.214</td>
<td>0.215</td>
<td>0.003</td>
</tr>
<tr>
<td>5.5</td>
<td>194.5</td>
<td>36.3</td>
<td>0.235</td>
<td>0.228</td>
<td>0.003</td>
<td>0.235</td>
<td>0.228</td>
<td>0.003</td>
</tr>
<tr>
<td>10</td>
<td>190</td>
<td>20</td>
<td>0.234</td>
<td>0.221</td>
<td>0.003</td>
<td>0.234</td>
<td>0.221</td>
<td>0.003</td>
</tr>
<tr>
<td>10</td>
<td>190</td>
<td>20</td>
<td>0.241</td>
<td>0.227</td>
<td>0.003</td>
<td>0.241</td>
<td>0.227</td>
<td>0.003</td>
</tr>
<tr>
<td>11.5</td>
<td>188.5</td>
<td>17.4</td>
<td>0.218</td>
<td>0.003</td>
<td>0.238</td>
<td>0.216</td>
<td>0.003</td>
<td>0.231</td>
</tr>
<tr>
<td>11.5</td>
<td>188.5</td>
<td>17.4</td>
<td>0.216</td>
<td>0.003</td>
<td>0.238</td>
<td>0.216</td>
<td>0.003</td>
<td>0.231</td>
</tr>
<tr>
<td>15</td>
<td>185</td>
<td>0.227</td>
<td>0.229</td>
<td>0.003</td>
<td>0.238</td>
<td>0.229</td>
<td>0.003</td>
<td>0.231</td>
</tr>
<tr>
<td>22</td>
<td>178</td>
<td>9.1</td>
<td>0.213</td>
<td>0.215</td>
<td>0.004</td>
<td>0.213</td>
<td>0.215</td>
<td>0.004</td>
</tr>
<tr>
<td>30</td>
<td>170</td>
<td>6.7</td>
<td>0.175</td>
<td>0.180</td>
<td>0.003</td>
<td>0.175</td>
<td>0.180</td>
<td>0.003</td>
</tr>
<tr>
<td>50</td>
<td>150</td>
<td>4</td>
<td>0.150</td>
<td>0.149</td>
<td>0.003</td>
<td>0.150</td>
<td>0.149</td>
<td>0.003</td>
</tr>
<tr>
<td>75</td>
<td>125</td>
<td>2.7</td>
<td>0.098</td>
<td>0.106</td>
<td>0.003</td>
<td>0.098</td>
<td>0.106</td>
<td>0.003</td>
</tr>
<tr>
<td>100</td>
<td>100</td>
<td>2</td>
<td>0.042</td>
<td>0.041</td>
<td>0.004</td>
<td>0.042</td>
<td>0.041</td>
<td>0.004</td>
</tr>
<tr>
<td>150</td>
<td>50</td>
<td>1.3</td>
<td>0.031</td>
<td>0.023</td>
<td>0.005</td>
<td>0.031</td>
<td>0.023</td>
<td>0.004</td>
</tr>
<tr>
<td>193</td>
<td>7</td>
<td>1.04</td>
<td>0.035</td>
<td>0.023</td>
<td>0.004</td>
<td>0.035</td>
<td>0.023</td>
<td>0.004</td>
</tr>
</tbody>
</table>

An initial set of experiments was performed without any collimation with increasing $r_s$ distances of 5.5, 11.5, 15, 30, 50, 75, 100, 150, 193 cm, and then a second set was performed with collimation at decreasing distances of 193, 150, 100, 75, 50, 22, 15, 10, 5.5, 0.5 cm. In some cases, there are duplicate images at some of the distances to ensure correct exposure, as shown in Table 6.3, which also shows phase contrast calculated after straightening for both edges, with $\gamma_{noA}$, representing the experiment performed without aperture collimation.

Images of the fibre at different $r_s$ and $r_d$ distances can be seen in Fig. 6.7 and with the associated line profiles in Fig. 6.8. As $r_s$ is systematically increased and $r_d$ correspondingly decreased, so that the magnification factor $M = \frac{r_s + r_d}{r_s}$ also decreases, the fibre becomes smaller but is easily visible until about 150 cm when it starts to become fainter. At $r_s=193$ cm and $r_d=7$ cm, the fibre is not visible and corresponds to an absorption type image as interference effects can not be seen when the detector is placed this close to the object. The particularly straight section of the fibre used
Figure 6.7: X-ray images of a single fibre with various magnification distances, at 30 kVp, and scanned at 25 µm resolution. The images for \( r_s = 100 \) cm and \( r_s = 150 \) cm show artifacts from the straightening program to the left of the image. For \( r_s = 193 \) cm, no fibre can be seen. This is equivalent to an absorption type image.

in these images was obtained by stretching it over a specially designed holder that enabled the straightening program to work well over all the magnifications used in the experiment. The line profiles reveal that the optimum range for \( r_s \) is between 10 and 22 cm, corresponding to magnifications between 20 and 10. This is reflected quantitatively in Fig. 6.9, where there is a peak at around 20 cm and then trails off gradually for larger \( r_s \) values. Interestingly, the set of measurements performed with collimation, consisting of two Pb apertures located at 33 cm and 195 cm from the source respectively, generally showed greater phase contrast values, except for two instances, than the un-collimated beam set of measurements. This would suggest that background scatter can influence
Figure 6.8: Associated line profiles through the images of Fig. 6.7 of a single fibre with various magnification distances.

This strong dependence on geometric distance was unfortunately not realized when performing earlier experiments, otherwise they would have been performed at this optimum $r_s$ distance, resulting in greater absolute phase contrast values. Nonetheless they were taken in the regime of around 85% of the optimum.
Figure 6.9: Phase contrast as a function of source to object distance with and without apertures, at 30 kVp, 100 µm (4 µm spot size) and scanned at 25 µm resolution.

Figure 6.10: Phase contrast as a function of magnification with and without apertures, at 30 kVp, 100 µm (4 µm spot size) and scanned at 25 µm resolution.
6.4 Phase contrast variation with filters

In clinical diagnostic x-ray practice, filters are used to remove lower energy x-rays from the beam to limit patient dose. This section investigates the way in which filters affect phase contrast. Since Al is commonly used in clinical practice, and was readily available, it is used here in a greater range of thicknesses than the other materials. Usually 2-3 mm of Al is used in practice [165], but since 2 mm reduced the phase contrast significantly, Al thicknesses between 0 and 2 mm were used to characterize this degradation. Other materials were used but only out of curiosity, and were not systematically or exhaustively studied.

![Image of X-ray images with line profiles](image)

Figure 6.11: X-ray images of fibres with various filter materials together with line profiles, 30 kVp, 100 µA (4 µm spot size), $r_x=55$ cm, $r_d=145$ cm and 50 µm scanner setting. Phase contrast values are shown in Fig. 6.15
Initial experiments used a grid of crossed fibres (Cuprophan RC 55) as the test object with a selection of filter materials in the beam positioned close to the source, with Pb apertures to reduce scattered radiation. Selected ROI of the images are shown in Fig. 6.11 together with a corresponding line profile averaged over the number of horizontal lines for comparison. As can be seen, the three vertical fibres vary in visibility and in their associated line profiles, however they can all be seen to reduce in clarity with the introduction of the filters of various types and thicknesses. The third fibre in particular, shows much greater phase contrast than the other two. A silicon filter with the same thickness (0.3 mm) as one of the aluminium filters, shows a similar reduction in phase contrast, as does 4.71 mm thickness of PMMA, while 0.94 mm Al reduces the phase contrast further and 2.00 mm Al nearly destroys phase contrast completely. These initial experiments were performed at 30 kVp tube potential, 100

![Grid of Cuprophan RC55 fibres imaged at 30 kVp, 100 μA, r_s=55 cm, 50 μm scan. No filter](image)

**Figure 6.12:** Grid of Cuprophan RC55 fibres used for imaging at 30 kVp, 100 μA (4 μm spot size), r_s=55 cm, r_d=145 cm at 50 μm scan without added filtration. The vertical fibres were used since the beam is narrower in this direction giving better phase contrast.
µA tube current and 50 micron setting on the scanner. The 50 micron setting is not as desirable for data resolution as the 25 micron setting, as the sharp phase peaks may occur between the data points. For reasons explained in Section 5.1.3, the 50 µm setting was initially used prior to when this data resolution problem became known. Furthermore the object was placed at $r_s=55$ cm due to the presence of other equipment in the enclosure at the time, and not only was it not optimum, but more of the fibres were included in the image. This was prior to the construction of a special clamp to hold and stretch the fibres which meant that more twisted and bent sections were included into the image which subsequently caused havoc with the fibre straightening program see Fig. 6.12. Therefore a more crude method of averaging limited sections of the image was used. To improve the phase contrast index statistics, 8 fibres were used and the average calculated over the number of scanned sections. The error in this case was determined as the standard error of the errors calculated in section 6.4.2.

A much larger section of the image showing all 8 vertical fibres is shown in Fig. 6.12, where it can be seen that it is difficult to find a straight 400 line section with good phase contrast on both sides. Therefore a variable section of lines from 10 to 400 was averaged and scanned down the entire 1512 lines of the image.

An example of phase contrast calculated in this way for sections of 50 averaged lines is shown in Fig. 6.13. The phase contrast for each section is shown in Fig. 6.14 for the case of no filtration where it can be seen that the maximum phase contrast occurs for sections of 10 averaged lines, due most likely to the non-uniformities in the fibre. The results of this analysis for images of the fibres with various filters, is shown in Table 6.4 and Fig. 6.15. A systematic decrease can be seen for phase contrast with increasing thickness of filter, particularly the thicker (0.94 mm and 2 mm) Al filters. Furthermore, Si and Al for the same thickness show similar phase contrast values indicating that similar Z materials have a similar affect on phase contrast, whereas a lighter material such as PMMA, of greater thickness, does not reduce phase contrast as much.
Figure 6.13: Line profiles for each section (50 lines) scanned across the image. Red circles indicate the maximum value for each fibre, and the cyan circles indicate the minimum values used for calculating phase contrast.

Figure 6.14: Phase contrast as calculated as the mean of the average number of lines in each scanned section for the no filter case, and the error in each case is the standard error.
Table 6.4: X-ray phase contrast index of a fibre with various filters obtained at 30 kVp, 100\(\mu\)A, \(r_s=55\) cm, \(r_d=145\) cm, 50 \(\mu\) detector setting.

<table>
<thead>
<tr>
<th>filter material</th>
<th>thickness</th>
<th>phase contrast (\gamma)</th>
<th>error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Be</td>
<td>0.05</td>
<td>0.129</td>
<td>0.002</td>
</tr>
<tr>
<td>Al</td>
<td>0.3</td>
<td>0.094</td>
<td>0.002</td>
</tr>
<tr>
<td>Al</td>
<td>0.44</td>
<td>0.090</td>
<td>0.002</td>
</tr>
<tr>
<td>Al</td>
<td>0.94</td>
<td>0.078</td>
<td>0.002</td>
</tr>
<tr>
<td>Al</td>
<td>2.0</td>
<td>0.076</td>
<td>0.002</td>
</tr>
<tr>
<td>Si</td>
<td>0.3</td>
<td>0.095</td>
<td>0.002</td>
</tr>
<tr>
<td>Au</td>
<td>0.02</td>
<td>0.118</td>
<td>0.002</td>
</tr>
<tr>
<td>PMMA</td>
<td>4.71</td>
<td>0.010</td>
<td>0.002</td>
</tr>
</tbody>
</table>

Figure 6.15: Phase contrast as a function of filter thickness, obtained at 30 kVp, 100\(\mu\)A, \(r_s=55\) cm, \(r_d=145\) cm, 50 \(\mu\) detector setting. Note for 0.3 mm Si and Al, the phase contrast is practically identical.
6.4.1 Aluminium grain size

To investigate whether the grain size of filter has an effect upon phase contrast some samples of pure aluminium were heated to disrupt the inherent grain size and then cooled at different rates, so that the samples would form either larger or smaller grain sizes. The actual size was not important, but only to determine whether the grain size of the aluminium filter had an effect upon phase contrast. From the better parts of each sample, a 5 cm$^2$ section was cut to use as the filter. A photograph of the various samples are shown in Fig. 6.16. Filters of the same thickness were imaged under identical conditions, first at 30 kVp, 100 $\mu$A and then at 60 kVp, 50 $\mu$A. The object used in this case was the finer PMMA step wedge, and although the phase contrast is not as strong as the fibre, it is enough to illustrate the case. X-ray images of the PMMA object with different filters are shown in Fig. 6.17.

![Aluminium filters with various grain sizes and thicknesses.](image-url)
Fig. 6.18 shows line profiles through the images for each filter. It can be easily observed that there is little variation between the profiles, showing negligible effect due to the grain size. A similar result is shown in Fig. 6.19 for the case of 60 kVp tube potential.

Calculation of the phase contrast for the best step which was between the air and the first PMMA step, taking into account the absorption contrast, is shown in Table 6.5, where it can be noticed that the phase contrast values for each grain size are within the error margins of each other. This indicates that filter grain size does not strongly influence phase contrast measurement.
Figure 6.18: Line profiles through PMMA step wedge using 2 mm various Aluminium filters at 30 kVp.

Figure 6.19: Line profiles through PMMA step wedge using 2 mm various Aluminium filters at 60 kVp.
Table 6.5: X-ray phase contrast for aluminium filter grain size for 1st step

<table>
<thead>
<tr>
<th>Grain size</th>
<th>phase contrast 30 kVp</th>
<th>error</th>
<th>phase contrast 60 kVp</th>
<th>error</th>
</tr>
</thead>
<tbody>
<tr>
<td>ordinary</td>
<td>0.050</td>
<td>0.009</td>
<td>0.05</td>
<td>0.01</td>
</tr>
<tr>
<td>small</td>
<td>0.057</td>
<td>0.009</td>
<td>0.04</td>
<td>0.01</td>
</tr>
<tr>
<td>large</td>
<td>0.056</td>
<td>0.009</td>
<td>0.05</td>
<td>0.01</td>
</tr>
</tbody>
</table>

6.4.2 Errors

A method of dealing with the errors in phase contrast calculation from x-ray images can be done as follows. For the case when there is no absorption, the phase contrast index, $\gamma$ is defined as the maximum minus the minimum, the difference, divided the maximum plus the minimum, the sum.

$$\text{phase contrast index } \gamma = \frac{\max - \min}{\max + \min} \quad (6.1)$$

It could equally well have been defined as the difference divided by the average, in which there is a factor of 2, but the above definition is more common and sufficient. For ease of mathematical expression, this definition is recast as

$$\gamma = \frac{a - b}{a + b} \quad (6.2)$$

Now the expectation of the variance of phase contrast $\gamma$ may be calculated as follows.

$$\text{Var}(\gamma) \approx \left( \frac{\partial \gamma}{\partial a} \right)^2 \text{Var}(a) + \left( \frac{\partial \gamma}{\partial b} \right)^2 \text{Var}(b) \quad (6.3)$$

$$\sigma_{\gamma}^2 = \frac{4b^2}{(a + b)^4} \sigma_a^2 + \frac{4a^2}{(a + b)^4} \sigma_b^2$$

$$= \frac{4}{(a + b)^4} \left( b^2 \sigma_a^2 + a^2 \sigma_b^2 \right)$$

$$= \frac{4}{(a + b)^4} \left( b^2 + a^2 \right) \sigma_a^2$$

$$\Rightarrow \sigma_{\gamma} = \frac{2}{(a + b)^2} \sigma_a \sqrt{b^2 + a^2}$$
with \( \sigma_a^2 \simeq \sigma_b^2 \) in the last step. Thus the error bars shown in the graphs are \( \sigma_\gamma \), when there is no or very little absorption.

The case when absorption is present changes the equation slightly, with an added term. Fig. 6.20 shows a sketch to illustrate the index calculation with \( a' \) and \( b' \) representing the difference in absorption levels, high and low respectively. There is now absorption contrast and phase contrast to consider so that the index is now modified.

![Figure 6.20: Illustration of phase contrast with absorption.](image)

\[
\gamma = \left( \frac{a - b}{a + b} \right) - \left( \frac{a' - b'}{a' + b'} \right) \tag{6.4}
\]

Calculating the variance of \( \gamma \) results in the following expression

\[
\text{Var}(\gamma) \approx \left( \frac{\partial \gamma}{\partial a} \right)^2 \text{Var}(a) + \left( \frac{\partial \gamma}{\partial b} \right)^2 \text{Var}(b) + \left( \frac{\partial \gamma}{\partial a'} \right)^2 \text{Var}(a') + \left( \frac{\partial \gamma}{\partial b'} \right)^2 \text{Var}(b')
\]

\[
\sigma_\gamma^2 = \frac{4b^2}{(a+b)^4}\sigma_a^2 + \frac{4a^2}{(a+b)^4}\sigma_b^2 + \frac{4b'^2}{(a'+b')^4}\sigma_{a'}^2 + \frac{4a'^2}{(a'+b')^4}\sigma_{b'}^2 \tag{6.5}
\]

\[
\approx \frac{4}{(a+b)^4} \left( b^2 + a^2 \right) \sigma_a^2 + \frac{4}{(a'+b')^4} \left( b'^2 + a'^2 \right) \sigma_{a'}^2
\]

with \( \sigma_a^2 \simeq \sigma_b^2 \) and \( \sigma_{a'}^2 \simeq \sigma_{b'}^2 \) in the last step. If a further assumption that \( \sigma_a^2 \simeq \sigma_{a'}^2 \), then this may be further simplified as follows

\[
\text{Var}(\gamma) \approx 4\sigma_a^2 \left( \frac{a^2 + b^2}{(a+b)^4} + \frac{a'^2 + b'^2}{(a'+b')^4} \right) \tag{6.6}
\]

\[
\Rightarrow \sigma_\gamma = 2\sigma_a \sqrt{\frac{a^2 + b^2}{(a+b)^4} + \frac{a'^2 + b'^2}{(a'+b')^4}}
\]
The errors shown in the tables and figures have been calculated via this method.

### 6.4.3 Filters and noise

It was noticed that imaging with filters seems to add more noise in a similar way to increasing the tube potential so that the images looked more ‘grainy’. The question that filters introduce extra noise to an image, thereby obscuring the phase contrast is difficult to answer, as separating this extra noise from the many existing sources of noise such as from the x-ray source, the image plate, as well as noise introduced by scanning and digitization is beyond the scope of this thesis.

One simple method to compare noise in the images is to take a region of interest and determine the mean and the standard deviation of a ROI of an image without any object detail or even better a blank image without an object. Since fluctuations in exposure make direct comparison difficult normalization is therefore used. Previous images for system characterization in chapter 5.1.4 can be used as a guide for different illumination differences. Each ROI can be evaluated in two directions, namely parallel and perpendicular to the scan direction. An example is shown in Fig. 6.21. These images were taken at the 50 µm setting on the scanner which is reflected by the roughly equal line profiles in each direction.

When blank images with filters, taken at 25 µm, are compared as shown in Fig. 6.22, a large difference for the standard deviation may be observed in the two directions due to the artifact caused by this setting on the BAS5000. Averaging parallel to the scan direction is relatively free from the artifact and useful for determining the noise occurring from filters.

The results of the mean versus standard deviation for a range of exposures and materials are shown in Fig. 6.23. The data points in blue and green circles represent the exposure data for the parallel and perpendicular directions at 50 µm resolution setting, while the coloured squares represent the Al filter materials and other filters as shown in
Figure 6.21: Blank x-ray images taken with 50 µm scan setting, with exposures of 30, 32 and 34 s with associated line profiles of the mean values for the ROI in directions parallel and perpendicular to the scan directions.

the legend, at 25 µm setting. It can be observed that the data falls into two categories, with the data in the upper part of the figure having higher standard deviation to mean values as a result of the scanning artifact at 25 µm parallel scan direction. The lower part of the figure shows a trend of the standard deviation increasing with increasing mean values as the square root of the mean, assuming a Poisson type distribution. There is a small difference between the unfiltered perpendicular (⊥) and parallel (||) scan directions and the Al filtered and unfiltered 25 µm perpendicular scan. However, since the filtered perpendicular 25 µm data has the same trend as the unfiltered as the 25 µm data, it may be concluded that the filter introduces no new noise component
Figure 6.22: Blank sections of x-ray images taken with 25 µm setting for the cases without a filter, 0.19 mm Cu and 0.38 mm Cu filters. Underneath are the associated line profiles, both parallel and perpendicular to the scan direction.

The same test can be made for noise increase for increasing tube potential. Although it seemed that the kVp experiment exhibited increased graininess with higher tube voltage, measurements of this suggests otherwise. The images for all kVp settings were made by trying maintain exposure rates within the dynamic range of the detector and at roughly similar brightness levels. Therefore there is no reduction in flux to increase the noise. As further evidence of this, the images were examined for noise levels by taking a region of the image without any detail. The mean and standard deviation were calculated in two directions as previously done and are shown in Fig. 6.24. The
Figure 6.23: Plot of normalized mean values versus standard deviation for parallel and perpendicular scan directions for both filtered and unfiltered x-ray images. Note the artifact caused by 25 µm scan setting when averaging parallel to the scan direction.

Differing psl brightness levels are evident in the last frame of the figure showing line profile means in the two directions. The respective standard deviations were measured and compared to the ones obtained for 50 µm scan at different exposure times as seen in Fig. 6.25. The trend of the kVp values is in keeping with the 50 µm scan (see Fig. 6.23) apart from the artifact, which is keeping with other 25 µm measured data. If more noise was introduced by higher kVp settings, one would expect the standard deviation to deviate from the previous trend which it does not. Therefore, the conclusion, particular in regards to phase contrast values, is that phase contrast is a maximum for lower kVp
Figure 6.24: Blank regions of the various kVp experiments. The line profiles in the last sub-figure show the absolute brightness levels of the images, averaged in parallel and perpendicular directions. The noisier profiles occur from the 25 µm scanning artifact tube potentials and is not the consequence of extra noise being introduced into the system from higher kVp settings.

Another method of analysis is to use the power spectrum and autocorrelation functions which are related via a Fourier transform by the Wiener-Khinchin theorem. Power spectral analysis captures the frequency content of a stochastic process and helps identify periodicities. The autocorrelation is the cross correlation of the signal, in this case the image, with itself. If the filter were to introduce a characteristic noise signal it may become visible by these means. The power spectrum analysis is shown in Fig. 6.26, for the case of an unfiltered image compared to one using a 0.38 mm Cu, while the autocorrelation calculation for various filtered and unfiltered cases are shown.
Figure 6.25: Measured mean and standard deviation for various kVp images plotted with earlier measurements. The kVp measurements are denoted by triangles.

in Fig. 6.27. The scan artifact is evident in Fig. 6.26, and in Fig. 6.27 a greater range of filters are compared in the direction parallel to the scan direction. As can be seen, both show little difference between filtered and unfiltered images.

### 6.5 X-ray spectrum

Simulations of x-ray spectra with filters of various materials and thicknesses show changes to the quality of the beam. The Feinfocus microfocus x-ray tube is similar to
conventional x-ray generators in producing x-rays from bombardment of a target with a high energy electron beam. The differences are in the way the beam is concentrated and in the shape of the target. Conventional tubes strike the flat target anode material at an angle, and the x-rays are emitted over a broad range of angles giving rise to the heel effect. Since x-rays are emitted from a range of depths below the surface of the anode, rays travelling a further distance are hardened by the target, and therefore the x-ray spectrum varies with the angle emitted from the target. In the case of the Feinfocus, the target is cylindrical, and therefore the angles are different from conventional targets which the simulation programs model. Nevertheless, the simulations may be instructive in qualitative differences to the beam by the addition of filters. Tungsten has strong K
Figure 6.27: Autocorrelation functions for various x-ray images with and without various filters in the direction parallel to the scan direction (i.e. without artifact).

lines at 59317.9, 57983.6, 67248.4 and 66957.3 eV, L lines at 8396.2 9671.4 9958.8 eV and M lines at 1775.6, 1773.3 and 1834.9 eV.

XOP (X-ray Oriented Program) was developed by the European Synchrotron Radiation Facility (ESRF) and Advanced Photon Source (APS) [166]. Fig. 6.28 shows the simulated spectra for various tube potentials for an x-ray tube generator with a tungsten target. Of particular interest are the characteristic K lines developing at about 80 kVp, superimposed over the broader bremsstrahlung curve. The peak of the bremsstrahlung curve shifts towards higher energies with increasing tube potential and much more flux is generated. No L lines are shown in this simulation. An initial hypothesis from these simulated spectrums was that phase contrast may have been
generated by the K lines, which would indicate that higher kVp settings should be preferred. However this was disproved by the kVp experiment which showed a decrease in phase contrast with increasing kVp. If the tube potential is kept at 30 kVp, and filters of various thicknesses of Al are introduced, the flux is reduced and the bremsstrahlung peak shifts slightly towards the higher energies, see Fig. 6.29.

Another simulation code, Xcomp5r was developed by Nowotny and Hyfer and is written as a DOS program in BASIC [167]. The spectra at 30 kVp for several filter materials and thicknesses is shown in Fig. 6.30. In contrast to the XOP program, it shows strong L series characteristic radiation which may influence phase contrast. A three dimensional plot is shown in Fig. 6.31. In the case of aluminium, it can be seen that the L peaks reduce in proportion to the thickness of the filter, while for the two copper filters, they disappear altogether.
Figure 6.29: Simulated spectra via XOP for 30 kVp with various Al filter thicknesses

Figure 6.30: Simulated spectra in using Xcomp5r for various filter materials at 30 kVp
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Since the spectra changes are an important component of this thesis and the simulations differed from one another, it was deemed worth measuring the actual spectra of the Feinfocus tube. This was accomplished by a solid state SiLi detector system, using a United Scientific Limited USC 514 Pulse Processor, mounted in a Tennelec Tennebin 3 rack, with a Tracor Northen TX 1236 Bias/Protection Module. This was connected to a WINEDS (Thomson Scientific Instruments) version 3.0 microanalysis system, see Fig. 6.32.

This detection system utilizes the absorption of x-rays by the Li doped Si crystal, where the energy deposited is proportional to the signal and recorded by a multichannel analyzer. Calibration of this type of system is required to determine the x-ray energy
relationship to the channel which is usually done with nuclear sources with accurately known energies [168]. There are a certain fraction events not recorded by the detector such as scattered radiation and characteristic secondary radiation out of the detector, often called the k-escape. Therefore there is some distortion of the ‘true’ spectrum. Nonetheless the measurements illustrate the changing nature of the spectrum with filter type and thickness.

All the measurements shown here have been scaled and shifted to give the best representation of the spectrum. Fig. 6.33 shows the spectrum at 30 kVp, 100 \(\mu\)A without any added filtration apart from the Be window at the source. In comparison to the simulations, three strong L lines can be seen from the microfocus source, similar to the Xcomp5r program. Successive figures (Fig. 6.34-Fig. 6.38) show how the spectrum changes for increasing Al thickness, with the first L line reducing in intensity until for 0.94 mm Al, all lines have gone completely.
For clarity the spectrum plots have been redone in colour and shown all together in Fig. 6.39 which highlights the diminishing L lines and the spectrum shift of the bremsstrahlung peak towards higher energies for each increase in Al thickness. For example, the unfiltered case shows roughly an average of 11-12 keV for the bremsstrahlung peak, while for the 0.94 mm Al filter, the average has shifted to around 20 keV.

6.6 Summary

Phase contrast as expected, was most pronounced for the smallest source size of 4 µm but also gave reasonable results at 6 µm (5% change) and 12 µm (15% change). At 25 µm the source produced multiple images of the fibre edge with 80% change in phase.
contrast, while at 50 µm, no phase contrast was observable. This is as expected since the ideal source size is a point source and larger source sizes will act to convolve the image, thereby reducing phase contrast.

A similar result was obtained with the lowest focussed tube potential of 30 kVp. Presumably lower voltages would have given better phase contrast, however in clinical settings higher voltages are preferred as they minimize dose. A dramatic reduction of around 45%, in phase contrast was observed for 60 kVp but it is likely the tube was not properly focussed since only a 30% reduction was observed for 90 kVp.

Phase contrast was found to vary with $r_s$ and $r_d$ distances with the optimum occurring around $r_s=20$ cm, $r_d = 180$ cm, corresponding to a magnification factor of around 10-13. This peak however was fairly broad with 85% of the optimum occurring between the ranges from 4 to 36.
When filters were introduced into the beam, phase contrast was found to reduce with thickness and atomic number. Filter orientation, smoothness and grain size did not affect phase contrast. Visually it appeared that filtered images looked more ‘grainy’ than unfiltered images as did the images obtained using higher tube potentials the 30 kVp images, however there appeared to be no increase in noise, except in the case of the 25 µm scan which introduced a scanning artifact.

The beam spectra was simulated and measured, showing strong L lines for the case of no added filtration. The L lines reduced as greater thicknesses of Aluminium were introduced into the beam, and the bremsstrahlung peak shifted towards higher energies. The cause of phase contrast loss with respect to beam filtration and imaging geometry is investigated in the simulation chapter 8.
Figure 6.36: Measured 30 kVp, 0.31 mm Al filter via WinEds program.
Figure 6.37: Measured 30 kVp, 0.45 mm Al filter via WinEds program.
Figure 6.38: Measured 30 kVp, 0.94 mm Al filter via WinEds program.
Figure 6.39: Measured x-ray spectrum with various Al filters.
Chapter 7

Refraction

This chapter examines the formation of phase contrast via ray tracing and refraction. It is simpler than the wave methods and is likely to give an initial crude estimate for calculating the effect of filters upon the image phase contrast. Nonetheless it is expedient in its comparative ease of simulation and hopefully will provide some gauge to the way filters act upon phase contrast in the image.

To accomplish this, the problem is divided into three parts. The first is to analytically calculate the path of the rays through the fibre to their eventual destination to the screen. The second part is to convert these ray positions into an intensity image, and the third part is to sum these intensities over the measured spectra to compare the filtered and unfiltered X-ray images.

Initially the refractive index of carbon is used as an approximation to the material of the fibre. This is later extended to the refractive index for cellulose reflecting the Cuprophan RC55 fibre composition. Then various combinations of air, cellulose and water are compared for the medium inside and outside the fibre.
7.1 Ray tracing

Determining the ray path through the fibre is similar to finding the transmission function for the Fresnel-Kirchhoff equation with the addition of keeping track of the angle changes. This can be implemented by two possible approaches. The first is to trace the path of each ray analytically and track its refraction changes at the fibre boundaries, and follow its trajectory to the detector screen. This is more tedious as it means determining all critical rays that delineate the various regions and writing separate code for each region, but executes faster than the second approach which is to pose the fibre as two concentric circles and to solve the quadratic equation for its intersection with each ray. This conceptually and aesthetically simpler method unfortunately suffers from long execution times on the order of ten fold compared to the first method and was not used for larger numbers of rays.

7.1.1 Analytical approach

Beginning with an angular density of rays with angle $\alpha$ emitted from the source, the angles are determined for various important rays through the fibre as shown in Fig. 7.1. The maximum angle, $\alpha_{\text{max}}$, that the rays can have to intersect the fibre can be calculated via the right angled triangle made by the tangent ray to the outer circle.

$$
\alpha_{\text{max}} = \arcsin \left( \frac{r_1}{r_s - r_1} \right)
$$

(7.1)

However, the angular spread of the rays is made twice as great as this to form a background for the intensity pattern. These rays are located on the detector screen by the straight forward tangent of the angle

$$
Y_{\text{mis}} = (r_s + r_d) \tan \alpha
$$

(7.2)
Some rays are totally externally reflected and are generally located well outside the geometrical projection of the fibre. As the ray density increases, rays less than but close to $\alpha_{\text{max}}$ possess this possibility. Let $\alpha_{\text{ext}}$ denote the critical angle at which total external reflection occurs. Text book theory shows that the refraction angle via Snell’s law [5] for an initial medium of air, from which the ray travels into a material with refractive index $n_{\text{mat}}$, is given by

$$\sin \theta_r = \frac{\sin \theta_i}{n_{\text{mat}}} \quad (7.3)$$

Relating this to the refractive index as discussed in the early chapters, $n = 1 - \delta + i\beta$, with minimal absorption so that $\beta$ may be neglected, this equation may be written as

$$\sin \theta_r = \frac{\sin \theta_i}{1 - \delta} \quad (7.4)$$

Figure 7.1: Some important rays through the fibre
Since the refractive index of the material is less than air for x-rays, there exists a critical angle of incidence for total external reflection when \( \sin \theta_r = 1 \), therefore

\[
\sin \theta_c = 1 - \delta \quad (7.5)
\]

For this angle, x-ray propagation is along the interface, and since \( \delta \ll 1 \), this only occurs for angles close to 90°. The incident and refracted rays must sum to 90°, therefore

\[
\sin(\frac{\pi}{2} - \theta_c) = 1 - \delta \quad (7.6)
\]

This can be written as in terms of cosine of the angle and expanding as a series as

\[
\cos \theta_c = 1 - \delta \quad (7.7)
\]

\[
1 - \frac{\theta_c^2}{2} + ... = 1 - \delta \quad (7.8)
\]

\[
\Rightarrow \theta_c \approx \sqrt{2\delta} \quad (7.9)
\]

Henceforth the critical angle \( \theta_c \) will be denoted as \( \theta_{c,ext} \) as there are more critical angles to be determined, plus it is desired to find an exact numerical value, dependent upon the geometry to be used in the algorithm. From Snell’s law, denoting the medium outside the fibre as \( n_{out} \), this angle is the inverse of the ratio of the indices as

\[
n_{out} \sin \theta_{c,ext} = n_{mat} \sin 90^\circ \quad (7.10)
\]

\[
\Rightarrow \theta_{c,ext} = \arcsin \left( \frac{n_{mat}}{n_{out}} \right)
\]
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To find the corresponding angle $\alpha_{c,ext}$ of the ray emitted from the source, the sine rule is used,

$$\frac{\sin \alpha_{c,ext}}{r_1} = \frac{\sin (\pi - \theta_{c,ext})}{r_s - r_1} = \frac{\sin \pi \cos \theta_{c,ext} - \cos \pi \sin \theta_{c,ext}}{r_s - r_1} = \frac{\sin \theta_{c,ext}}{r_s - r_1}$$

$$\Rightarrow \alpha_{c,ext} = \arcsin \left( \frac{r_1 \sin \theta_{c,ext}}{r_s - r_1} \right) = \arcsin \left( \frac{r_1 n_{mat}}{(r_s - r_1) n_{out}} \right)$$

When $n_{mat}$ is of the order of $1 - 10^6$, this is an extremely small angle and only becomes apparent when the angle density is high enough to include angles between $\alpha_{c,ext} \leq \alpha < \alpha_{max}$. Rays with these angles will be reflected with an angle equal to the incidence angle, $\theta_r = \theta_i = \theta_{ext}$. To find the location of these rays at the detector, another angle $\beta$ is introduced as shown in Fig. 7.2, where $\beta = \pi - \alpha - (\pi - \theta_{i}) = \theta_{i} - \alpha$, $\theta_i = \arcsin \left( \frac{(r_s-r_1)}{r_1} \sin \alpha \right)$. The new angle to the detector, can be calculated from the straight line of the normal as $\alpha_{new} = \pi - \theta_r - \beta$ and to determine the position of the ray on the screen, the intersection of the ray with the outer circle is required, $(x, y)$.

Using the angle $\beta$, and the radius of the outer circle $r_1$, this intersection is $x = r_1 \cos \beta$ and $y = r_1 \sin \beta$. Now the position on the screen may be calculated as

$$Y_{reflected} = (x + r_1 + r_d) \tan (\alpha_{new}) + y$$

(7.12)

For rays with angles less than $\alpha_{c,ext}$, there are two more regions to consider. One region in which the ray traverses the fibre wall only, and the other where the rays traverse the interior of the fibre. These two regions are delineated by a tangent to the inner circle. A ray that meets the exterior circle undergoes refraction at the boundary. The angle of incidence $\theta_{in,wall}$ can be found via the sine rule.
Figure 7.2: Rays with angle $\theta_{ext}$, reflected by the fibre wall, $\theta_r = \theta_i = \theta_{ext}$

\[
\frac{\sin \alpha_{wall}}{r_1} = \frac{\sin(\pi - \theta_i)}{r_s - r_1} = \frac{\sin \pi \cos \theta_i - \cos \pi \sin \theta_i}{r_s - r_1} = \frac{\sin \theta_i}{r_s - r_1} \Rightarrow \sin \alpha_{wall} = \arcsin \left( \frac{r_1}{(r_s - r_1) \sin \theta_i} \right) \tag{7.13}
\]

Upon entering the fibre wall, the ray is refracted to $\theta_r$ and meets the inner circle
at a tangent via

\[ n_{out} \sin \theta_i = n_{mat} \sin \theta_r \]  \hspace{1cm} (7.14)

but by right angle triangle

\[ \sin \theta_r = \frac{r_2}{r_1} \]  \hspace{1cm} (7.15)
therefore

\[
\sin \alpha_{\text{wall}} = \arcsin \left( \frac{r_1}{r_s - r_1} \frac{n_{\text{mat}}}{n_{\text{out}}} \sin \theta_r \right)
\]

\[
= \arcsin \left( \frac{r_2}{r_s - r_1} \frac{n_{\text{mat}}}{n_{\text{out}}} \frac{r_1}{r_2} \right)
\]

\[
\Rightarrow \alpha_{\text{wall}} = \arcsin \left( \frac{r_2}{r_s - r_1} \frac{n_{\text{mat}}}{n_{\text{out}}} \right)
\]

Therefore for \( \alpha_{\text{wall}} \leq \alpha \leq \alpha_{\text{ext}} \), the rays will traverse the fibre wall only, and for rays between \(-\alpha_{\text{wall}} < \alpha < \alpha_{\text{wall}}\), the rays will traverse the interior of the fibre. Rays traversing the wall possess symmetrical angle changes at the boundaries. To calculate the position on the screen these rays travel to, the intersection of the ray leaving the outer circle is calculated as \((x, y)_{\text{leaving}}\)

\[
Y_{\text{wall}} = (r_1 + r_d - x_{\text{leaving}}) \tan(\pi - \gamma - \beta) + y_{\text{leaving}}
\]

For the rays traversing the hollow interior, a few more angle changes are required, see Fig. 7.4. Fortunately, there is symmetry to simplify the calculation. The refraction angle \( \theta_{ro} \) of the entering ray at the outer circle is calculated as before. This ray then enters the inner circle, and this angle of incidence \( \theta_{ih} \) is determined using the sine rule again.

\[
\frac{\sin(\pi - \theta_{ih})}{r_1} = \frac{\sin \theta_{ro}}{r_2}
\]

\[
\Rightarrow \delta = \pi - \theta_{ro} - (\pi - \theta_{ih})
\]

The angle \( \delta \), subtended by the two radii \( r_1 \) and \( r_2 \) may be calculated via \( \delta = \pi - \theta_{ro} - (\pi - \theta_{ih}) \). This will be used later to determine the new angle to the screen. The ray is refracted again at the boundary by Snell’s law

\[
n_{\text{mat}} \sin \theta_{ih} = n_{\text{in}} \sin \theta_{rh}
\]
The ray then crosses the interior of the fibre, subtending an angle $\pi - 2\theta_{ro}$, and intersects the inner circle by symmetry, with angle $\theta_{rh}$. It undergoes refraction at the boundary into the fibre wall

$$n_{in} \sin \theta_{rh} = n_{mat} \sin \theta_{ih} \quad (7.20)$$

It traverses the fibre wall material until meeting the outer circle, subtending angle $\delta$, then enters the wall with an angle by symmetry $\theta_{ro}$, and refracted at this boundary into $\theta_{io}$. To calculate the new angle upon leaving the fibre, all that is required is to first compute the angle $\phi = \pi - \beta - 2\delta - (\pi - 2\theta_{ro})$. Thus the new angle to the screen is then given by $\phi - \theta_{io}$.

Figure 7.4: Rays traversing the hollow interior of the fibre
Now there is a question of the density of rays to use. The finer the spacing of rays, the more realistic the intensity profile will be, however this requires more memory space and execution time, both of which are limited. The approach taken here was to keep increasing the density of rays until the computing resources were either exhausted or no more information was gained by further processing. The following figures show the progression of increasing ray density and decreasing refractive index.

![Figure 7.5: Refraction pattern via ray tracing for 20 rays and the index of refraction of the fibre $n_{\text{mat}}=0.99$. The cyan lines are the rays that miss the fibre which is coloured red. The darker blue lines are the rays that traverse the interior of the fibre, and inside the fibre they are coloured black. The lines in green are the rays that traverse the fibre wall.](image)

Starting with only 20 rays for illustration, as shown in Fig. 7.5, and using an artificial refractive index of $n_{\text{mat}} = 0.99$, it useful to examine the ray pattern. The rays traversing the hollow interior are hardly deviated, and the rays that miss the fibre are undeviated. Only the rays that traverse the fibre wall show deviation. The angular spacing in this case is not fine enough to have any reflected rays. Next 100 rays are shown, in Fig. 7.6, which has a finer spacing to enable more rays to traverse the fibre wall. Some of these interior rays that are close to the wall are deviated by comparatively greater angles.
Thus a gap in the rays is developed which is the mechanism of contrast, even though there is no absorption. However, it is not until 1000 rays are used (Fig. 7.7), that reflected rays and wall rays become numerous. The deviations near the fibre edges are enough to show the rough image formation. Using a more physically realistic refractive index of \( n_{\text{mat}} = 0.99999 \) and 1000 rays, the refraction pattern is shown in Fig. 7.8. Here the deviation is so small that it is not discernable. Using a large enough distance to the detector \( r_d \), the rays separate enough to allow distinction near the geometrical projection of the edges as shown in Fig. 7.9. Although greater numbers of rays were used in calculation of the intensity patterns in the next section such as \( 10^5 \) and \( 10^6 \), these can not be displayed due to memory limitations of the system.

### 7.2 Intensity profile

One simple method of calculating the intensity profile, is to divide the screen array into a number of bins, and to count the number of rays falling into each bin. A better
Figure 7.7: Refraction pattern via ray tracing for 1000 rays and the index of refraction of the fibre $n_{\text{mat}}=0.99$. In this case some of the rays traversing the wall (green) in the upper part of the figure are obscured by the order in which the rays were plotted. The magenta coloured lines are the rays that have been totally externally reflected.

Figure 7.8: Refraction pattern via ray tracing for 1000 rays and the index of refraction of the fibre $n_{\text{mat}}=0.99999$. This is a fairly realistic pattern, since the refractive decrement of the fibre material is in this order, and hence the refraction effects are very small.
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Figure 7.9: Entire refraction pattern via ray tracing for 1000 rays and the index of refraction of the fibre $n_{\text{mat}}=0.99999$. This is a fairly realistic pattern, since the refractive decrement of the fibre material is in this order, and hence the refraction effects are very small. The concentration of the rays through the fibre wall (green) opens a gap to the interior rays (navy blue) that delineate the walls of the fibre.

way, though, is to consider that the energy deposited onto the screen as distributed between the rays. For example, if the angular spread between two successive rays is small, say falling into one bin, then all of the energy is deposited into this bin. If however it is spread across multiple bins, then the energy deposited is proportional to the distance between the rays and the number of bins it falls across. The reflected rays for example, are spread widely apart and therefore their energy is deposited across many bins is small. The wall refracted rays by contrast are concentrated around the geometrical projection of the fibre, resulting in a much greater deposition of energy. Adjacent to these concentration of rays is a void with no rays which has the effect of further accentuating the boundary, as shown previously in Fig. 7.9. The intensity pattern for various ray densities is shown in Fig. 7.10. Using 1000 rays with $10^{-4}$ m resolution results in a coarse intensity profile. As the number of rays increases and the corresponding spacing between the rays becomes smaller, a peak can be seen to develop either side of the fibre edge. The times for these calculations are shown in
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Figure 7.10: Intensity pattern for various numbers of rays from $10^3$ to $10^6$ and resolutions, with the index of refraction of the fibre $n_{\text{mat}}=0.99999$. The blue plot is the histogram of the rays giving an intensity in counts, while the green is the distributed energy.

Table 7.1. The first calculation takes longer than the second in this case due to the computer cache which enables faster successive calculations. The last calculation takes about 15 minutes to calculate the energy intensity pattern on an AMD 64 X2 dual core processor 3800+ 2.01 GHz with 1 GB RAM desktop machine and does not show any extra information. As a comparison to the Fresnel diffraction calculation presented in the next chapter, these take 11 hours! Demonstrating the expediency of the ray tracing method. Therefore, since the second case shows a physically realistic looking pattern, i.e. for $10^4$ rays with $10^{-5}$ resolution and these are considered sufficient for spectrum calculations. Since these plots are for a single energy only they are not representative of the fibre image until the entire spectrum is used, although they appear similar. Too many rays will increase the execution time when done over an entire spectrum and may not be necessary from physical constraints which will be examined in the next chapter. At this stage, as a first approximation, physical realism is the guiding principle until otherwise determined.

The peak asymmetry in Fig. 7.10 is thought to be an artifact of the display or
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<table>
<thead>
<tr>
<th>Rays</th>
<th>Resolution</th>
<th>Ray trace time</th>
<th>Intensity calculation time</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^3$</td>
<td>$10^{-4}$</td>
<td>0.234 s</td>
<td>1.953 s</td>
</tr>
<tr>
<td>$10^4$</td>
<td>$10^{-5}$</td>
<td>0.203 s</td>
<td>0.344 s</td>
</tr>
<tr>
<td>$10^5$</td>
<td>$10^{-6}$</td>
<td>1.187 s</td>
<td>11.218 s</td>
</tr>
<tr>
<td>$10^6$</td>
<td>$10^{-7}$</td>
<td>10.312 s</td>
<td>907.203 s</td>
</tr>
</tbody>
</table>

Table 7.1: Table of calculation times

<table>
<thead>
<tr>
<th>Energy(keV)</th>
<th>$f_1$</th>
<th>$f_2$</th>
<th>$n = 1 - \delta + i\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>6.012689408</td>
<td>0.0058933016</td>
<td>0.9999958400 + i*0.000000004</td>
</tr>
<tr>
<td>11</td>
<td>6.010413636</td>
<td>0.0047396989</td>
<td>0.999996563+i*2.709942653e-009</td>
</tr>
<tr>
<td>20</td>
<td>6.002227188</td>
<td>0.0011729506</td>
<td>0.999998962+i*2.028684266e-010</td>
</tr>
<tr>
<td>30</td>
<td>6</td>
<td>0.00044254</td>
<td>0.999999539+i*3.401768406e-011</td>
</tr>
</tbody>
</table>

Table 7.2: Table of $f_1$, $f_2$ and refractive index $n$ values of carbon for selected energies. Note how small the $\beta$ values are which are ignored in the refraction calculations.

perhaps an uneven splitting of the number of rays between the upper and lower halves of the fibre. Since it is not present on the displays for $10^4$ but only on the higher number of rays, it is most likely due to the display properties of Matlab. Since the following chapter presents the more rigorous Fresnel diffraction model, it was considered minor and not worth investigating.

Some $f_1$ and $f_2$ values for carbon [146] with the corresponding calculated index of refraction for some specific energies are shown in Table 7.2. Linear interpolations were used between given tabulated energy values. Line intensity profiles for these $n$ values, are shown in Fig 7.11, where it can be observed that as the energy increases, the phase peak profile sharpens becoming narrower as the refractive index decreases. Interestingly, the profiles show higher peak values at the edges for the lower energies, due to the larger phase decrement. Simulated images of these intensity profiles are shown in Fig. 7.12 where the width of the refraction peaks can be seen to contract more easily. The differing brightness levels between the images are due to the Matlab function, `pcolor`, that was used to display the images. This assigns the minimum and maximum elements of the matrix to the first and last colors in the colormap. The remaining elements in matrix are assigned colours or in this case shades of grey by a
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Figure 7.11: Intensity pattern for various energies for carbon. Notice as the energy increases, the profile narrows.

Figure 7.12: Simulated images via the intensity pattern for various energies for carbon.
7.3 Energy spectra

Now that the intensity profiles have been calculated for various energies, it is required to calculate and sum them over an entire energy range of the spectra for both filtered and unfiltered images. Measured spectra from chapter 5.5 for two cases are tested. One without filtration and the other with the maximum of 0.94 mm of aluminium. The previously measured spectrum Fig. 6.39 is reproduced here Fig. 7.13, showing the spectra for various Al filter thicknesses, with the greatest spectral difference occurring for the 0.94 mm Al filter and no filter cases. This involves taking the 1075 energies of the measured spectra and ray tracing for each associated refractive index and calculating the intensity profiles for each energy and summing the 1075 profiles together. As the number of rays increases, the calculation time also increases. For 1000 rays with $10^{-4}$ m resolution, Fig. 7.14 shows the comparison for filtered and unfiltered line profiles, while Fig. 7.15 shows the same comparison using $10^4$ rays. Increasing the number of rays to $10^5$ rays with 1 μm resolution improves the detail but does not change the
Figure 7.14: Calculated line profiles and images via ray tracing for filtered (0.94 mm Al) and unfiltered spectrums using 1000 rays and $10^{-4}$ resolution.

Overall shape of the line profiles and shows no further detail. The calculation time for this took 6.7 hours per spectrum and is seen in Fig. 7.16. Notice that the pattern becomes more refined the greater the number of rays, and that the filtered image and line profile, have narrower phase contrast peaks and become slightly larger when normalized. The interesting conclusion from this is that there is little difference in phase contrast between filtered and unfiltered x-ray refracted images. The difference occurs in a slight change to the shape of the peaks with the filtered image profile possessing narrower peaks, particularly in the darker negative peak.

### 7.4 Cellulose

The previous refraction patterns were based on $f_1$ and $f_2$ values for carbon for simplification, however the cuprophan fibre is made of regenerated cellulose (cellulose...
Figure 7.15: Calculated line profiles and images via ray tracing for filtered (0.94 mm Al) and unfiltered spectrums using 10 000 rays and $10^{-5}$ m resolution

Figure 7.16: Calculated line profiles and images via ray tracing for filtered (0.94 mm Al) and unfiltered spectrums using 100 000 rays and $10^{-6}$ m resolution
II), which is a thermodynamically more stable form of natural cellulose (cellulose I), with the chemical formula \([C_6H_{10}O_5]_n\), where \(n\) can vary from 500 to 5000 depending on the source of the polymer [169]. Cuprophan gets its name from the process of spinning hollow fibres from solutions of cellulose in a cuprammonium complex [170].

The measured density varies between 1.27 – 1.61 g/cm\(^3\) [171] due to the complexities of measurement and is the subject of current and past research [172], [173], [174]. Using an arbitrary density of 1.560 g/cm\(^3\), the \(f1\) and \(f2\) values used in this thesis have been calculated by the weighted sum from the elemental composition. The values differ slightly in comparison to carbon and are shown graphically in Fig. 7.17 and as a check the \(\delta\) and \(\beta\) values so derived were compared to the online calculator provided by Henke [175] which are shown in Fig. 7.18. There is excellent agreement except for some of the higher energies in the absorption, \(\beta\), values but since \(\beta << \delta\) these differences are ignored in the simulation as only the real part of the refractive index was used.

The corresponding \(\delta\) and \(\beta\) values along with log values for carbon and cellulose are shown in Fig. 7.19.
Figure 7.18: Calculated phase, $\delta$, and absorption, $\beta$, values from weighted sum of individual elements of cellulose from NIST [176] data and online calculated tables of Henke [175]

Figure 7.19: Comparison of calculated $\delta$ and $\beta$ values for carbon (NIST) and cellulose $[C_6O_5H_{10}]_n$
Figure 7.20: Calculated line profiles and images for cellulose via ray tracing for filtered (0.94 mm Al) and unfiltered spectrums using 10,000 rays and $10^{-5}$ m resolution.

Simulated images for filtered and unfiltered cases using $10^4$ rays can be seen in Fig. 7.20 and using $10^5$ rays in Fig. 7.16. The resulting figures are very similar to those calculated with carbon.

### 7.4.1 Combinations of refractive materials

Changing the medium outside and inside the fibre leads to some interesting simulations. The real and imaginary parts of the refractive indices are shown in Fig. 7.21. Filling the interior with water for example gives a refraction pattern in Fig. 7.22. The peak heights are reduced by comparison with air, showing that in this case it would be more difficult to discern the edges by phase contrast alone, and slightly better when the beam is unfiltered ($\gamma = 0.86$ versus $\gamma = 0.75$).

The converse of water outside air inside gives the intensity pattern shown in
Figure 7.21: Calculated real $\delta$ and imaginary $\beta$ values for comparison for carbon, cellulose ($C_6H_{10}O_5$), water ($H_2O$) and air ($\approx78.10\%N_2,20.98\%O_2,0.93\%Ar$)

Figure 7.22: Calculated line profiles and images via ray tracing for air outside the fibre, water inside, for filtered (0.94 mm Al) and unfiltered spectrums using 10 000 rays and $10^{-5}$ m resolution. Unfiltered image has phase contrast of 0.86, while the filtered image has 0.75
Figure 7.23: Calculated line profiles and images via ray tracing for water outside the fibre, air inside, for filtered (0.94 mm Al) and unfiltered spectrums using 10,000 rays and $10^{-5}$ m resolution. The profiles have a phase contrast index of $\gamma = 0.996$ and 0.991 respectively.

Fig. 7.23, shows similar contrast to the case where both mediums are air, with similar phase peak heights for both spectrums (0.996 and 0.991 respectively). If both the interior and exterior media is water, then a large difference occurs with the unfiltered spectrum giving better contrast (0.93) than the filtered case (0.76) as shown in Fig. 7.24.

Turning the hollow fibre into a solid cellulose fibre gives the refraction patterns shown in Fig. 7.25, which by comparison shows poorer contrast to the hollow case with either filtered or unfiltered spectrums. This correlates with experiment where hollow fibres showed much better phase contrast than solid fibres see Fig. 5.29.

7.5 Summary

This chapter has provided an initial means of simulating x-ray phase contrast of fibres with the two extreme cases of no filter and 0.94 mm Al filter. The normalized line
Figure 7.24: Calculated line profiles and images via ray tracing for water inside and outside the fibre, for filtered (0.94 mm Al) and unfiltered spectrums using 10 000 rays and $10^{-5}$ m resolution. $\gamma = 0.93, 0.76$ respectively

Figure 7.25: Calculated line profiles and images via ray tracing for air outside and solid cellulose fibre, for filtered (0.94 mm Al, $\gamma = 0.24$) and unfiltered spectrums ($\gamma = 0.31$) using 10 000 rays and $10^{-5}$ m resolution
profiles show similar peak heights for both cases with the main difference being the width of the peaks. When sufficient density of rays are used, the negative peaks have a minimum of zero giving a phase contrast of unity for both spectrums. Observable differences in filtering the spectrum results in a narrower phase peak, both positive (lighter) and negative (darker) peaks.

The binning parameter acts in a similar way to detector resolution and hence changing this parameter would alter the heights of the detected intensity peaks and hence the phase contrast. However, there is no inability to resolve the patterns where the peaks are narrow. This section was not meant to be exhaustive but as a precursor to the more rigorous Fresnel theory. Therefore, the chosen resolution and number of rays used has been fixed in a similar way to the resolution of a detector would be fixed.

Experimenting with filling the fibre void with water does not improve detectability as in fact it seems to decrease the phase peaks, and a solid fibre reduces the peaks even further. This could be further investigated but since air was used in the experimental section it is more expedient to check the simulation with the wave method which is content of the next chapter.
Chapter 8

Diffraction simulations

This chapter outlines basis of the wave optical simulations beginning with the Fresnel-Kirchhoff representation using plane waves incident upon a single edge. This is the basis of the step wedge experiments and assuming a semi-infinite edge, can be simplified using Fresnel integrals for efficient calculation. The phase shift introduced by the edge variance in the $\xi$ direction can be represented by the transmission function $q(\xi)$. In effect, the transmission function is treated as a one dimensional projection of the edge. Subsequently, it is generalized to the case of spherical incident waves on a fibre. The fibre however, is modelled as a two dimensional cross section of a hollow cylinder with the path length through the walls as the variable for the phase shift difference. The simplest case is to position the transmission plane on the exit side of the fibre. Placing the object plane in the middle of the fibre was also investigated, but did not yield useful mathematical expressions and due to the extra complexity, was not used in the simulation programs.

It is common in the literature to model the three dimensional nature of the fibre as a two dimensional cross section due to the simplicity of expression, and then to further treat the transmission function as a one dimensional variable so that $q(\xi, \eta)$ becomes effectively $q(\xi)$; Monin et al. [42], Kardjilov et al. [177], Arfelli et al. [178],
Chen et al. [179], El-Ghazaly et al. [180], Pogany et al. [65], Cowley [96]. However, this simplification not often justified, since for spherical waves $q(\eta)$ is not insignificant. As a starting point to building a simulation program as a test of the experiment, this point was initially overlooked, but found to lead to a problem in the Fresnel-Kirchhoff formulation of the diffraction integral.

Rather than make ad hoc assumptions to make the Fresnel-Kirchhoff integral separable, it was decided to use the less accurate Fresnel theory, which although not strictly accurate across the entire width of the diffraction pattern, is sufficiently accurate near the edge, to enable the transmission function $q(\xi, \eta)$, to be separated into $q(\xi)q(\eta)$. Since the object is uniform in the $\eta$ direction, $q(\eta)$ is a very slowly varying function compared to $q(\xi)$ and can be essentially considered as constant, and this scaling factor may now be brought outside of the integral.

Computer calculations based on the Fresnel theory produced simulations much closer to experiment than the Fresnel-Kirchhoff calculations. Importantly though, they reveal that contrast degradation when filters are used, is ultimately, but not solely a matter of a spectral change. Even though the filter causes the x-ray spectrum to shift towards higher energies, these higher energies only cause the peaks in the diffraction pattern to ‘narrow’ by dispersion in the fibre rather than to decrease, resulting in very little amplitude change of the phase peaks compared to the unfiltered pattern. However, when other processes in the image chain such as: the energy efficiency of the image plate, the effect of reading the image plate by the scanning laser beam of the scanner and thirdly, the effect of source size are also included in the process, these affect the filtered diffraction pattern more so than the unfiltered pattern. The narrower peaks of the filtered pattern are smoothed more than the broader unfiltered pattern. This decrease in phase contrast follows the trend as observed in experiments.
8.1 Fresnel-Kirchhoff formulation

The simplest case for modelling the Fresnel-Kirchhoff equation is to use an incident plane wave upon a straight edge which is both partially absorbing and refracting. This simplifies the integrals so that appropriate Fresnel Sine and Cosine integrals can be used to reduce the calculation considerably. For the case of the fibre and a point source, the equation is modified and the fibre is modelled as a hollow cylinder and the transmission function is calculated as a function of the variable $\xi$ assuming the $\eta$ dependence can be ignored. The equation is then evaluated by direct integration using sufficient sampling of the Fresnel zones across the fibre.

8.1.1 Fresnel-Kirchhoff formulation in 1 dimension

The Fresnel-Kirchhoff integral for the wave amplitude at the image location $(x, y)$, for plane incident wave in Cowley’s [96] notation where $k = 1/\lambda$, is

$$\psi(x, y) = \frac{i}{2\lambda} \int \int q(\xi, \eta) \frac{e^{-2\pi ikr}}{r} \left( 1 + \cos \mathbf{Z} \cdot \mathbf{r} \right) d\xi d\eta$$

(8.1)

where $q(\xi, \eta)$ is the object transmission function at the object plane $(\xi, \eta)$ and $(1 + \cos \mathbf{Z} \cdot \mathbf{r})$ is the obliquity factor which for very small angles is approximated as 2. Modifying this for spherical incident wave, and the usual notation ($k = 2\pi/\lambda$), the integral becomes

$$\psi(x, y) = \frac{i}{2\lambda} \int \int \frac{e^{-iks}}{s} q(\xi, \eta) \frac{e^{-ikr}}{r} d\xi d\eta$$

(8.2)

For a source located $r_s$ from transmission plane $(\xi, \eta)$, and image plane $(x, y)$ located a further $r_d$, by geometry the following two relations can be formed

$$s = \sqrt{r_s^2 + \xi^2 + \eta^2}$$

$$\approx r_s + \frac{\xi^2 + \eta^2}{2r_s}$$

(8.3)


\[ r = \sqrt{r_d^2 + (x - \xi)^2 + (y - \eta)^2} \]  
\[ \approx r_d + \frac{(x - \xi)^2 + (y - \eta)^2}{2r_d} \]  

(8.4)

These will replace the values in the exponents in the integrals, but the denominator can be simply approximated by \( s \approx r_s, r \approx r_d \). Therefore the integral becomes,

\[
\psi(x, y) = \frac{i}{\lambda} e^{-ik(r_s + r_d)} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{e^{-i \frac{(x-\xi)^2}{2r_s}}}{r_s r_d} q(\xi, \eta) e^{-i \left[ \frac{(x-\xi)^2 + (y-\eta)^2}{2r_d} \right]} d\xi d\eta
\]  

(8.5)

Following Cowley, if the transmission function \( q(\xi, \eta) \) varies only appreciably in one direction, say \( \xi \), then this integral may be separated.

\[
\psi(x, y) = A \int_{-\infty}^{\infty} e^{-i \frac{(x-\xi)^2}{2r_s}} q(\xi) e^{-i \frac{(r_s + r_d)(x-\xi)^2}{2r_d}} d\xi \int_{-\infty}^{\infty} e^{-i \frac{(y-\eta)^2}{2r_s}} e^{-i \frac{(r_s + r_d)(y-\eta)^2}{2r_d}} d\eta
\]  

(8.6)

The integral over \( \eta \) may now be evaluated as a Gaussian function by manipulating the exponent into a perfect square. Taking the exponent of this integral

\[
-ik \left( \frac{\eta^2}{2r_s} \right) - i \left[ \frac{(y - \eta)^2}{2r_d} \right] 
\]
\[
= -\frac{ik}{2} \left[ \frac{\eta^2 r_d + (y^2 - 2y\eta + \eta^2) r_s}{r_s r_d} \right] 
\]
\[
= -\frac{ik}{2r_s r_d} \left( r_s + r_d \right) \left( \eta^2 - \left[ \frac{2yr_s}{r_s + r_d} \right] \eta + \left[ \frac{yr_s}{r_s + r_d} \right]^2 - \left[ \frac{yr_s}{r_s + r_d} \right]^2 + y^2 r_s \right) 
\]
\[
= -\frac{ik(r_s + r_d)}{2r_s r_d} y^2 r_s - \left( \frac{ik(r_s + r_d)}{2r_s r_d} \right) \times \left( -\left[ \frac{yr_s}{(r_s + r_d)} \right] \right)^2 - \frac{ik(r_s + r_d)}{2r_s r_d} \left( \eta - \frac{yr_s}{(r_s + r_d)} \right)^2 
\]

\[
\equiv B \quad \text{independent of } \eta
\]

This enables the integral to now be written as

\[
\psi(x, y) = Ae^B \int_{-\infty}^{\infty} e^{-i \frac{(x-\xi)^2}{2r_s}} q(\xi) e^{-i \left[ \frac{(x-\xi)^2}{2r_d} \right]} d\xi \int_{-\infty}^{\infty} e^{-i \left( \frac{r_s + r_d}{2r_s r_d} \right) \left( \eta - \frac{yr_s}{(r_s + r_d)} \right)^2} d\eta
\]

(8.8)
Taking the exponent in the $\eta$ integral, and denoting $M = \frac{r_s + r_d}{r_s}$

\[
-\frac{ik(r_s + r_d)}{2r_s r_d} \left( \eta - \frac{yr_s}{r_s + r_d} \right)^2 = \frac{-ikM}{2r_d} \left[ \eta - \frac{y}{M} \right]^2
\]  

(8.9)

Using the well known Gaussian integral value

\[
\int_{-\infty}^{\infty} e^{-ax^2} \, dx = \sqrt{\frac{\pi}{a}}
\]

the shift in the exponent, $\eta - \frac{y}{M}$, does not change the shape or value of this integral, and hence the constant, $a$, may be equated to $\frac{ikM}{2r_d}$. The integral over $\eta$ can then be shown to yield

\[
\int_{-\infty}^{\infty} e^{-\eta^2} \, d\eta = \sqrt{\frac{\pi}{ikM}}
\]

\[
= \sqrt{\frac{r_d\lambda}{M^2}} \quad \text{using} \quad k = \frac{2\pi}{\lambda}
\]

These four manipulations above can be verified by careful contour integration. Putting this altogether, the diffraction integral becomes

\[
\psi(x) = \frac{i}{\lambda} \frac{e^{-ik(r_s + r_d)}}{r_s r_d} \sqrt{\frac{r_d r_s \lambda}{(r_s + r_d)i}} \int_{-\infty}^{\infty} e^{-ik\left(\frac{\xi^2}{2r_s}\right)} q(\xi) e^{-ik\left[\frac{(x-\xi)^2}{2r_d}\right]} \, d\xi
\]

\[
= \sqrt{\frac{ir_s r_d}{\lambda(r_s + r_d)}} \frac{e^{-ik(r_s + r_d)}}{r_s r_d} \int_{-\infty}^{\infty} e^{-ik\left(\frac{\xi^2}{2r_s}\right)} q(\xi) e^{-ik\left[\frac{(x-\xi)^2}{2r_d}\right]} \, d\xi
\]

8.1.2 Incident plane wave on an edge

The plane wave can be described as $e^{-k \cdot r}$ where $k$ is the wavevector. Wavelets in the Huygens style are created at the boundaries which propagate to the detecting plane. The Fresnel-Kirchhoff equation for a plane wave in one dimension, given by Cowley [96],
but with \( k = 2\pi/\lambda \) is

\[
\psi(x) = \sqrt{\frac{i}{r_d\lambda}} e^{-ikr} \int_{-\infty}^{\infty} q(\xi)e^{-\frac{ikr}{2r_d}(x-\xi)^2} d\xi
\] (8.10)

This may also be written with \((x - \xi)^2\) interchanged with \((\xi - x)^2\) as

\[
\psi(x) = \sqrt{\frac{i}{r_d\lambda}} e^{-ikr} \int_{-\infty}^{\infty} q(\xi)e^{-\frac{ikr}{2r_d}(\xi-x)^2} d\xi
\] (8.11)

For a transmission function \( q(\xi) \) of the form

\[
q(\xi) = \begin{cases} 
1 & \text{if } \xi \geq a, \\
- \frac{\phi}{k\delta\tau} - \frac{\mu/2}{k\beta} & \text{if } \xi < a.
\end{cases}
\] (8.12)

where \( \tau \) is the thickness of the step. The term \( k\delta \) can be replaced by \( \phi/\tau \), the phase change of the wave and \( k\beta \) can be written in terms of the attenuation coefficient \( \mu \) as \( \mu/2 \), the absorption. This requires breaking the integral into separate parts and further manipulation into Fresnel Sine (\( S \)) and Cosine (\( C \)) integrals reduces the calculation considerably.

\[
\psi(x)
\]

\[
= \sqrt{\frac{i}{r_d\lambda}} e^{-ikr_d} \left\{ \int_{-\infty}^{a} e^{-i\phi-\frac{\mu}{2}\tau} e^{-\frac{ikr_d(\xi-x)^2}{2r_d}} d\xi + \int_{a}^{\infty} e^{-\frac{ikr_d(\xi-x)^2}{2r_d}} d\xi \right\}
\]

\[
= \sqrt{\frac{i}{r_d\lambda}} e^{-ikr_d} \left\{ e^{-i\phi-\frac{\mu}{2}\tau} \int_{-\infty}^{a} e^{-\frac{ikr_d(\xi-x)^2}{2r_d}} d\xi + \int_{a}^{\infty} e^{-\frac{ikr_d(\xi-x)^2}{2r_d}} d\xi \right\}
\]

using variable change

\[
u = \sqrt{\frac{k}{\pi r_d}} (\xi - x)
\] (8.14)

\[
\Rightarrow \quad du = \sqrt{\frac{k}{\pi r_d}} d\xi
\]

and \( u_a = \sqrt{\frac{k}{\pi r_d}} (a - x) \)
\[ \psi(x) = \sqrt{\frac{i}{r_d \lambda}} e^{-ikr_d} \left\{ e^{-i\phi - \frac{u^2}{2}} \int_{u = -\infty}^{u_a} e^{-i\pi \frac{u^2}{2}} \sqrt{\frac{\pi r_d}{k}} du + \int_{u_a}^{\infty} e^{-i\pi \frac{u^2}{2}} \sqrt{\frac{\pi r_d}{k}} du \right\} \]

\[ = \sqrt{\frac{i}{2}} e^{-ikr_d} \left\{ 1 - \left( e^{-i\phi - \frac{u^2}{2}} \right) \left( \frac{1}{2} - \frac{i}{2} \right) + \left( e^{-i\phi - \frac{u^2}{2}} - 1 \right) [C - iS] \left[ \sqrt{\frac{k}{\pi r_d}} (a - x) \right] \right\} \]

For example, a PMMA step height of 1 mm, thickness 1 mm with \( r_s = 0.25, r_d = 1.75 \) at 10 keV energy produces a phase change of \( \phi = -146 \) rad/mm and absorption coefficient of 0.371/mm and the line profile across an edge is shown in Fig. 8.1. This was calculated with 10 000 points across the image screen position, and shows the transition of a line profile between the darker step and the air. The profile shows similarities to the experimental PMMA step-wedge profiles in chapter 5 (see Fig. 5.11). The simulation shows multiple fringes for one energy calculation, but when extended for real spectrums, such as for an unfiltered and a 0.94 mm Al filtered spectra, the resulting profiles smooth out these multiple fringes as shown in Fig. 8.2. These were calculated for a step-wedge consisting of 2 steps, of 1 and 2 mm, for both thickness and
Figure 8.2: Fresnel-Kirchhoff simulation calculated using planar incident wave for a step PMMA object of 1 and 2 mm height and thickness, with $r_s = 0.055$, $r_d = 1.945$ at 30 keV energy, unfiltered 0.94 mm Al filtered beam and 10 000 points across the image plane. See 8.3 for a magnified view of the edges.

height. The two line profiles are similar in that the phase peaks are of roughly equal magnitude, except that the filtered spectrum shows reduced absorption. Magnified portions of these steps are shown in Fig. 8.3 illustrating the comparison more fully.

However, contrary to experiment, phase contrast is increased for the filtered case due to the reduced absorption, $\gamma_{filt} = 0.47$ while $\gamma_{unfilt} = 0.46$. While the approximation of an incident plane wave is reasonable for the distances and wavelengths considered, the mixture of phase and absorption contrast is an apparent problem, as the filter hardened spectra will attenuate less than the unfiltered case. This is addressed using the Cuprophan RC55 fibre, for which the attenuation is negligible and next section deals with the extension from plane to spherical incident waves.
Figure 8.3: Magnified portions of Fresnel-Kirchhoff simulation calculated using planar incident wave for a step PMMA object of 1 and 2 mm height and thickness, with \( r_s = 0.055 \), \( r_d = 1.945 \) at 30 keV energy, unfiltered 0.94 mm Al filtered beam and 10 000 points across the image plane.

### 8.1.3 Spherical Waves

A more realistic description is an extension from plane waves to incident spherical waves. The geometry in this case is more complex, and the projected thickness of the object changes with the \( \xi \) coordinate, as shown in Fig. 8.4. The transmission function is now a function of \( \xi \),

\[
q(\xi) = \begin{cases} 
  e^{t(1 + \frac{\xi^2}{2r_s^2})} & \text{for } 0 \leq \xi < h \\
  e^{r_s(\frac{\xi}{r}-1)+t(1+\frac{\xi^2}{2r_s^2})} & \text{for } h \leq \xi < \frac{rh}{r_d} \\
  1 & \text{for } \xi \geq h
\end{cases}
\]
where $h$ is the height of the step, $t$ is the thickness, $R$ is the distance of the source to the object plane. The integral calculation must be split into three components and is long and tedious and will be omitted. A more useful result, since absorption by the step-wedge is still present, is to determine the transmission function for a fibre as considered in the following section.
8.1.4 Fresnel-Kirchhoff equation for a long straight cylinder

A hollow cylindrical fibre as a cross section may be represented geometrically by two concentric circles in the plane. The transmission function is dependent upon the distance through the fibre to the object plane which is placed on the exit side. The spherical wave from the source is modified by the presence of the fibre, modelled as the 1-D projected phase change along $\xi$, and from this plane, a secondary source of spherical waves is emitted towards the detector (image) plane. In the absence of the fibre, the incident spherical wave can be described by

$$e^{-ikR} = e^{-ik(R-L_1-\varepsilon)-ikL_1-ik\varepsilon}$$  \hspace{1cm} (8.16)

where $L_1$ is the distance through an imaginary circle representing the fibre, $\varepsilon$ is the distance from the circle to the $\xi$ axis, and $R$ is the total distance from the source to $\xi$ axis. The presence of a solid fibre with path length $L_1$, alters this to

$$\frac{e^{-ikR}}{R} = \frac{e^{-ik(R-L_1-\varepsilon)-ikL_1-ik\varepsilon}}{R}$$

$$= \frac{R}{e^{-ik(R-L_1)} \cdot e^{-iknL_1}}$$

$$= \frac{R}{e^{-ikR} \cdot e^{-ik(n-1)L_1}}$$  \hspace{1cm} (8.17)

The length $L_1$ through the solid cylinder may be described in terms of $\varepsilon$, $r_s$ and $r_1$

$$L_1 = 2\sqrt{r_1^2 - (r_s - r_1)^2} \frac{\varepsilon^2}{\varepsilon^2 + r_s^2}$$  \hspace{1cm} (8.18)

Using this equation (eq. 8.18) and substituting for $R$.

$$\frac{e^{-ik\sqrt{\xi^2 + r_s^2}} \cdot e^{-ik(n-1)^2 \sqrt{r_1^2 - (r_s - r_1)^2} \frac{\varepsilon^2}{\varepsilon^2 + r_s^2}}}{\sqrt{\xi^2 + r_s^2}}$$  \hspace{1cm} (8.19)

It is an easy matter to extend this now to a hollow cylinder as shown in Fig. 8.5. The
Figure 8.5: Fibre geometry schematic with fibre before object axis.

The hollow part of the figure can be treated as an extra cylinder with a path length through it denoted as $L_2$

$$e^{-i k \sqrt{\xi^2 + r_s^2}} \cdot e^{-ik(n-1) \left[ 2 \frac{r_s^2 - (r_s - r_1)^2}{\sqrt{\xi^2 + r_s^2}} - 2 \frac{r_s^2 - (r_s - r_1)^2}{\sqrt{r_s^2 + r_s^2}} \right]}$$

$$\frac{1}{\sqrt{\xi^2 + r_s^2}}$$

(8.20)
The full Fresnel-Kirchhoff equation through the fibre then becomes

$$
\psi(x) = K \int_{-\infty}^{\infty} \frac{e^{-ikr_q}}{r_q} q(\xi) e^{-ikr} \left[ 2\sqrt{r_1^2 - (r_s - r_1)^2} \frac{\xi^2}{\xi^2 + r_s^2} - 2\sqrt{r_2^2 - (r_s - r_2)^2} \frac{\xi^2}{\xi^2 + r_s^2} \right] d\xi
$$

$$
\times \frac{e^{-ik(\xi-x)^2}}{\sqrt{r_d^2 + (\xi-x)^2}} d\xi
$$

(8.21)

where $K$ is a scaling constant. The transmission function $q(\xi)$ is then

$$
q(\xi) = e^{-ik(n-1)^2[t_1-t_2]}
$$

(8.22)

where

$$
t_1 = \sqrt{r_1^2 - (r_s - r_1)^2} \frac{\xi^2}{\xi^2 + r_s^2}
$$

$$
t_2 = \sqrt{r_2^2 - (r_s - r_2)^2} \frac{\xi^2}{\xi^2 + r_s^2}
$$

(8.23)

(8.24)

The full path length $2(t_1 - t_2)$ as a function of $\xi$, is shown in Fig. 8.6, is particularly sharp near the edges, and is thought to be responsible for the excellent phase contrast.
obtained with a fibre compared to an edge. The edge by comparison has only a constant value across the domain of the object transmission plane. Methods of solving this equation Eq. 8.21, fall into two groups: direct integration or via approximation by Fresnel Integrals.

8.1.5 Direct integration of Fresnel-Kirchhoff equation

The dependence of the transmission function $q(\xi)$ on the object plane variable $\xi$, unfortunately means that Fresnel Sine and Cosine integrals can not be used to simplify the calculation. Consequently, integration from $-\infty$ to $\infty$ across the object ($\xi$) plane is too numerically expensive. Fortunately, this range may be reduced by modifying the Fresnel-Kirchhoff integral in the following manner. Starting with the Fresnel-Kirchhoff definition as,

$$
\psi(x) = K \int_{-\infty}^{\infty} \frac{e^{-ikr_q}}{r_q} q(\xi) \frac{e^{-ikr}}{r} d\xi
$$

(8.25)

with the transmission function $q(\xi)$ defined generally for the moment as

$$
q(\xi) = \begin{cases} 
q(\xi) & \text{for } |\xi| < a \\
1 & \text{for } |\xi| \geq a 
\end{cases}
$$

then expanding Eq. 8.25, and adding an extra term and subtracting it again such that the equation is unchanged.

$$
\psi(x) = K \left\{ \int_{-\infty}^{-a} \frac{e^{-ikr_q}}{r_q} \frac{e^{-ikr}}{r} d\xi + \int_{-a}^{a} \frac{e^{-ikr_q}}{r_q} q(\xi) \frac{e^{-ikr}}{r} d\xi + \int_{a}^{\infty} \frac{e^{-ikr_q}}{r_q} \frac{e^{-ikr}}{r} d\xi - \int_{-a}^{a} \frac{e^{-ikr_q}}{r_q} \frac{e^{-ikr}}{r} d\xi \right\}
$$

(8.26)
This is in effect a Babinet style representation, which upon relevant grouping becomes

\[
\psi(x) = K \left\{ \int_{-\infty}^{\infty} \frac{e^{-ikr}}{r} \frac{e^{-ikr}}{r} d\xi + \int_{-a}^{a} \frac{e^{-ikr}}{r} q(\xi) \frac{e^{-ikr}}{r} d\xi - \int_{-a}^{a} \frac{e^{-ikr}}{r} \frac{e^{-ikr}}{r} d\xi \right\}
\]

\[
= K \left\{ \int_{-\infty}^{\infty} \frac{e^{-ikr}}{r} d\xi + \int_{-a}^{a} \frac{e^{-ikr}}{r} \left[q(\xi) - 1\right] \frac{e^{-ikr}}{r} d\xi \right\} \tag{8.27}
\]

The first part of this expression \( K \int_{-\infty}^{\infty} \frac{e^{-ikr}}{r} d\xi \) can be equated as a spherical wave from the source to the detector \( \frac{e^{-ikR}}{R} \), where \( R = r_s + r_d \), so that

\[
\psi(x) = \frac{e^{-ikR}}{R} + \Psi(x) \tag{8.28}
\]

Instead of integrating over an infinite range, it has now been reduced to \([-a, a]\).

### 8.1.6 Fresnel zones

For integration across the fibre, it is necessary to determine the number of Fresnel zones. The distance from the source is \( L = \sqrt{r_s^2 + \xi^2} \) and the distance to the detector is \( L' = \sqrt{r_d^2 + \xi^2} \), the path difference at the position \( \xi \) is \( \Delta L = L + L' - r_s - r_d \). The phase difference is then

\[
\Delta \phi = \frac{2\pi}{\lambda} \Delta L \tag{8.29}
\]

\[
= \frac{2\pi}{\lambda} \left( \sqrt{r_s^2 + \xi^2} - r_s \right) + \frac{2\pi}{\lambda} \left( \sqrt{r_d^2 + \xi^2} - r_d \right)
\]
Letting $\Delta \phi = n\pi$ and rearranging to find $\xi$ gives

\[
n\pi = \frac{2\pi}{\lambda} \left( \sqrt{r_s^2 + \xi^2} - r_s + \sqrt{r_d^2 + \xi^2} - r_d \right)
\]

\[
\Rightarrow \frac{n\lambda}{2} = \sqrt{r_s^2 + \xi^2} - r_s + \sqrt{r_d^2 + \xi^2} - r_d
\]

\[
\approx r_s \left( 1 + \frac{\xi^2}{2r_s^2} \right) + r_d \left( 1 + \frac{\xi^2}{2r_d^2} \right) - r_s - r_d
\]

\[
= \frac{\xi^2}{2} \left( \frac{r_s + r_d}{r_s r_d} \right)
\]

\[
\Rightarrow \xi = \sqrt{\frac{n\lambda r_s r_d}{r_s + r_d}}
\]

Therefore successive position radii for a $\pi$ phase change are $\xi_n \approx \sqrt{n\lambda r_s r_d}$. The distance between these is

\[
\xi_{n+1} - \xi_n = \sqrt{\frac{(n+1)\lambda r_s r_d}{r_s + r_d}} - \sqrt{\frac{n\lambda r_s r_d}{r_s + r_d}}
\]

\[
= \frac{1}{\sqrt{r_s + r_d}} \left[ n \left( 1 + \frac{1}{n} \right) \lambda r_s r_d \left( \frac{1}{n} + \frac{1}{n^2} \right) - \left[ n\lambda r_s r_d \right]^{1/2} \right]
\]

\[
\approx \frac{1}{\sqrt{r_s + r_d}} \left[ n\lambda r_s r_d \right]^{1/2} \left( 1 + \frac{1}{2n} \right) - \left[ n\lambda r_s r_d \right]^{1/2}
\]

\[
= \frac{\left[ n\lambda r_s r_d \right]^{1/2}}{2n\sqrt{r_s + r_d}}
\]

\[
= \frac{1}{2} \sqrt{\frac{\lambda r_s r_d}{n(r_s + r_d)}}
\]

Therefore the spacings vary as $\frac{1}{\sqrt{n}}$. At 10 keV, the fibre width corresponds to about 7000 zones, and for $r_s = 0.055$ m, the smallest spacing is about $3 \times 10^{-8}$ m. Sampling uniformly so that the smallest interval is sampled twice gives $\frac{216 \times 10^{-8} m}{3 \times 10^{-8} m} \times 2 \approx 14000$ points to be integrated. For 30 keV, this becomes 24300 points. An example of this type of calculation is shown in Fig. 8.7, where the line profile is calculated for 10 000 points integrated across the object plane, while Fig. 8.8 is calculated for 100 000 points. Neither of these line profiles are realistic compared to the experimental images. Investigating as to why the one dimensional formulism of the Fresnel-Kirchhoff
Figure 8.7: Fresnel-Kirchhoff simulation of a fibre image at 10 keV, with 10 000 points across the object plane.

Figure 8.8: Fresnel-Kirchhoff simulation of a fibre image at 20 keV, with 100 000 points across the object plane.
integral gives erroneous line profiles, it is useful to look at the form of the transmission function in one and two dimensional spaces as shown in Fig. 8.9. In two dimensions, the transmission function \( q(\xi, \eta) \), has a more complicated form. The distance \( t_1 \) through outer part of the fibre can be written as

\[
t'_1 = \sqrt{r_1^2 - \frac{\xi^2 \left( \sqrt{r_s^2 + \eta^2} - r_1 \right)^2}{r_s^2 + \xi^2 + \eta^2}}
\]  

(8.30)

where \( r_1 \) is the radius of the outer circle. Likewise the inner part is described by

\[
t'_2 = \sqrt{r_2^2 - \frac{\xi^2 \left( \sqrt{r_s^2 + \eta^2} - r_1 \right)^2}{r_s^2 + \xi^2 + \eta^2}}
\]  

(8.31)

where \( r_2 \) is the radius of the inner circle. The transmission function is then

\[
q(\xi, \eta) = e^{ik(n-1)^2(t'_1-t'_2)}
\]  

(8.32)

Written explicitly it is

\[
q(\xi, \eta) = e^{ik(n-1)^2\left(\sqrt{r_1^2 - \frac{\xi^2 \left( \sqrt{r_s^2 + \eta^2} - r_1 \right)^2}{r_s^2 + \xi^2 + \eta^2}} - \sqrt{r_2^2 - \frac{\xi^2 \left( \sqrt{r_s^2 + \eta^2} - r_1 \right)^2}{r_s^2 + \xi^2 + \eta^2}}\right)}
\]  

(8.33)

Compared to the 1D form repeated below

\[
q(\xi) = e^{ik(n-1)^2\left(\sqrt{r_1^2 - \frac{\xi^2 \left( \sqrt{r_s^2 + \eta^2} - r_1 \right)^2}{r_s^2 + \xi^2 + \eta^2}} - \sqrt{r_2^2 - \frac{\xi^2 \left( \sqrt{r_s^2 + \eta^2} - r_1 \right)^2}{r_s^2 + \xi^2 + \eta^2}}\right)}
\]  

(8.34)

The effective path length corresponding to the phase mask of \( q(\xi, \eta) \) is shown in Fig. 8.9. The variation in the \( \eta \) direction is almost constant compared to the \( \xi \) direction, and indicates that the approximation of \( q(\xi, \eta) \) as \( q(\xi) \) is reasonable. However, the phase is more important \( k(n-1)^2(t_1 - t_2) \), as demonstrated by Fig. 8.10, which shows the phase of \( q(\xi, \eta) \) and again for practical purposes, is a constant in the \( \eta \) direction over
many wavelengths. Therefore the scaling constant $K$ may not be correct. It appears that the background level in Fig. 8.7 and Fig. 8.8 is too low, suggesting a problem in reducing the 2D integral to one dimension. Many attempts were made to try and remedy the situation by artificially raising the background level, trying to solve the 2D integral over a limited arbitrary range in the $\eta$ direction, and searching the literature for alternative methods such as Snigirev et al [61] which is discussed in the next section, but all to no avail. The spherical wavefront may be changing by too many wavelengths over the $\xi$ range compared to the distortion introduced by the fibre.

8.2 Fresnel-Kirchhoff for smaller fibres

In a paper by Snigirev et al [61] an expression is derived for the Fresnel-Kirchhoff formulation in which it has been reduced to a one dimensional equation to
In the \( \eta \) direction over 10 times the range of the \( \xi \) axis, the phase is virtually constant.

The above equation is recast in

\[
E(x_1, y_1) = \frac{1}{\sqrt{i\lambda r_0 r_1}} e^{\frac{2\pi i}{\lambda} \left( r + \frac{(y_1 - y_0)^2}{2r_0} \right)} \int dx e^{\frac{2\pi i}{\lambda} \left( r + \frac{(x - x_0)^2 + (x - x_1)^2}{2r_1} \right)} e^{i\varphi(x)}
\]  

(8.35)

where \( r_0 \) and \( r_1 \) are the source-to-object and object-to-hologram distances. They have defined distances somewhat differently as used here since they model a synchrotron source with \( r_0 \) being of the order of 40 m. Also \((x_1, y_1)\) in their case represents the detector plane and \((x_0, y_0)\) represents the source plane. The object, in this case also a fibre, is located at the plane \((x, y)\) with the long axis of the fibre orientated along the \( y \)-axis which alters the phase of the wavefield by \( \varphi(x) \). The above equation is recast in
the following form

$$E(x_1, y_1) = E(x_0, y_0)(1 + c(x_1))$$

(8.36)

where $c(x_1)$ is responsible for the image formation of the fibre and explicitly it is

$$c(x_1) = \sqrt{\frac{r}{i\lambda r_0 r_1}} e^{\frac{2\pi i}{\lambda} \left(-\frac{(x_1-x_0)^2}{2r_0}\right)} \int_{-R}^{R} dx e^{\frac{2\pi i}{\lambda} \left(r + \frac{(x-x_0)^2}{2r_0} + \frac{(x-x_1)^2}{2r_1}\right)} \left[e^{i\varphi(x)} - 1\right]$$

(8.37)

which is very similar to the method done in this thesis by restricting the range of integration. The corresponding intensity normalized against the background is

$$I(x_1) = 1 + 2\text{Re}[c(x_1) + |c(x_1)|^2]$$

(8.38)

These last two equations were used for simulation in their paper, the results of which are shown in Fig. 8.11 and Fig. 8.12. These simulations are repeated here explicitly for comparison. Using the same distances, but at 10 keV for convenience, results in the following line profiles as shown in Fig. 8.13 and Fig. 8.14. This energy produced the most similar results to Snigirev et al, even though there were some small calculation differences. Snigirev used the method of stationary phase to perform the integrals whereas they have been integrated directly here. Also the refractive index was slightly different in this case as the refractive index was calculated here from the tabulated form factors for individual elements of cellulose. Despite these differences the line profiles are remarkably similar which indicates the robustness of the method. These
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Figure 8.12: Fresnel-Kirchhoff calculated line profiles from Snigirev et al for 10 µm $r_0=40$ m and $r_1=0.5$ and 2.00 m fibre.

Figure 8.13: Fresnel-Kirchhoff calculated directly line profiles for 10 µm solid fibre at 10 keV, $r_0=40$ m and $r_1=0.25$ and 0.3 m fibre.

Figure 8.14: Fresnel-Kirchhoff calculated directly line profiles for 10 µm solid fibre at 10 keV, $r_0=40$ m and $r_1=0.5$ and 2.00 m fibre.
parameters were then changed to those used in the thesis, first of all with the same distances as Snigeriv et al, but with a hollow fibre as shown in Fig. 8.15 and Fig. 8.16, from which it can be seen that they are not too different from the solid fibre case. Then changing the distances systematically, by decreasing \( r_0 \) and increasing \( r_1 \) and calculating the line profiles for the case of a solid fibre as shown in Fig. 8.17 and then for a hollow fibre as shown in Fig. 8.18. As can be seen, they both begin to oscillate for distances \( r_0=0.05 \) m and \( r_1=1.95 \) m and wildly for \( r_0=0.05 \) m and \( r_1=1.95 \) m. A similar phenomena occurs if the fibre diameter is increased to the experimental size as used in this thesis i.e. 100 \( \mu \)m with 8 \( \mu \)m wall thickness as shown in Fig. 8.19. These were all calculated for 100 000 points across the object plane and 10 000 points across the image plane, i.e. very high resolution taking the order of about 5 minutes per profile. Oscillatory integrals are notoriously difficult to evaluate and the problem is not due to the theory nor implementation of the theory, since for small fibres the results correlate with Snigirev. It is most likely due to numerics but whether instability or roundoff errors is not known. This is however is not a problem for the Fresnel method as presented in the next section.
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Figure 8.16: Fresnel-Kirchhoff calculated directly line profiles for 10 µm hollow fibre at 10 keV, \( r_0 = 40 \) m and \( r_1 = 0.50 \) and 2.00 m fibre

Figure 8.17: Fresnel-Kirchhoff calculated directly line profiles for 10 µm solid fibre at 10 keV for distances as indicated

Figure 8.18: Fresnel-Kirchhoff calculated directly line profiles for 10 µm hollow fibre at 10 keV for distances as indicated
Figure 8.19: Fresnel-Kirchhoff calculated directly line profiles for 100 μm hollow fibre at 10 keV for distances as indicated

8.3 Fresnel formulation

The basic assumptions used are that the scalar wave approximation is valid and that obliquity factor is small enough to be ignored. For the Fresnel formulation, the spherical wavefronts emitted by the source are approximated by parabolic wavefronts over the region of interest.

The Fresnel approximation was derived earlier (Eq. 3.57) and can be stated as

\[
f(x, y, z) = \frac{e^{ikz}}{i\lambda z} e^{i\frac{\pi}{\lambda z}(x^2+y^2)} F \left( \frac{x}{\lambda z}, \frac{y}{\lambda z} \right)
\]  

(8.39)

where \( f(x, y, z) \) replaces the field \( U(x, y, z) \) and \( F \) is the Fourier transform of the field at \( f(x, y, 0) \) represented by

\[
F(p, q) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y, 0) e^{i\frac{\pi}{\lambda z}(x^2+y^2)} e^{-i2\pi(px+qy)} dx dy
\]  

(8.40)

This time not using separate coordinate systems for the object plane and image plane and instead denoting the object as located at position \( (x, y, 0) \), see Fig. 8.20, at a distance \( D \) from the point source and the image plane located at a further distance at
In the absence of the fibre, substituting Eq. 8.41 into the Fourier transform equation, Eq. 8.40 gives

$$F_0(p, q) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ikD} \frac{e^{i\pi}(x^2+y^2)}{D} e^{-i2\pi(px+qy)} \, dx \, dy$$

$$= \frac{e^{ikD}}{D} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{i\frac{\pi}{2}(\frac{1}{D} + \frac{1}{z})} (x^2+y^2) e^{-i2\pi(px+qy)} \, dx \, dy$$  \hspace{1cm} (8.42)
Now defining the following substitutions

\[ x_0 = \frac{\lambda p}{\left(\frac{1}{D} + \frac{1}{z}\right)} \]
\[ y_0 = \frac{\lambda q}{\left(\frac{1}{D} + \frac{1}{z}\right)} \] (8.43)

The exponent of the exponential in Eq. 8.42 can be rearranged as

\[
i\frac{\pi}{\lambda}\left(\frac{1}{D} + \frac{1}{z}\right) (x^2 + y^2) - i2\pi(px + qy)
= i\frac{\pi}{\lambda}\left(\frac{1}{D} + \frac{1}{z}\right) \left[ x^2 + y^2 - \frac{2\lambda}{\left(\frac{1}{D} + \frac{1}{z}\right)}(px + qy) \right] \] (8.44)

So that the part inside the square brackets may be formed into a perfect square.

\[
x^2 + y^2 - \frac{2\lambda}{\left(\frac{1}{D} + \frac{1}{z}\right)}(px + qy) + \left(\frac{\lambda p}{\left(\frac{1}{D} + \frac{1}{z}\right)}\right)^2 - \left(\frac{\lambda q}{\left(\frac{1}{D} + \frac{1}{z}\right)}\right)^2 - \left(\frac{\lambda q}{\left(\frac{1}{D} + \frac{1}{z}\right)}\right)^2
= \left[ x - \frac{\lambda}{\left(\frac{1}{D} + \frac{1}{z}\right)} p \right]^2 + \left[ y - \frac{\lambda}{\left(\frac{1}{D} + \frac{1}{z}\right)} q \right]^2 - \lambda^2\left(\frac{1}{D} + \frac{1}{z}\right)^2(p^2 + q^2)
= [x - x_0]^2 + [y - y_0]^2 - [x_0^2 + y_0^2] \] (8.45)

Hence the Fourier transform equation, Eq. 8.42 without the fibre, denoted as \( F_0 \) becomes

\[
F_0(p, q) = \frac{e^{ikD}}{D} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{i\frac{\pi}{D}\left[\frac{1}{D} + \frac{1}{z}\right](x^2 + y^2)} e^{-i\frac{\pi}{D}\left[\frac{1}{D} + \frac{1}{z}\right](x_x^2 + y_y^2)} dx dy
= \frac{e^{ikD}}{D} e^{-i\frac{\pi}{D}\left[\frac{1}{D} + \frac{1}{z}\right](x_x^2 + y_y^2)} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{i\frac{\pi}{D}\left[\frac{1}{D} + \frac{1}{z}\right](x^2 + y^2)} dx dy \] (8.46)

Transforming this equation into polar coordinates via \( r^2 = (x - x_0)^2 + (y - y_0)^2 \),
allows the integral to be evaluated as

\[ F_0(p, q) = e^{ikD} D e^{-i\pi \lambda \left(\frac{1}{D} + \frac{1}{z}\right)} \int_{r=0}^{\infty} e^{\frac{i\pi}{\lambda z} (x_0^2 + y_0^2)} r dr d\theta \]

\[ = e^{ikD} D e^{-i\pi \lambda \left(\frac{1}{D} + \frac{1}{z}\right)} \int_{r=0}^{\infty} e^{\frac{i\pi}{\lambda z} (x_0^2 + y_0^2)} i\lambda \frac{1}{D} + \frac{1}{z} \] (8.47)

Substitution of Eq. 8.47 into Eq. 8.39 yields

\[ f_0(x, y, z) = e^{ikD} \int_{r=0}^{\infty} e^{\frac{i\pi}{\lambda z} (x_0^2 + y_0^2)} F_0 \left( \frac{x}{\lambda z}, \frac{y}{\lambda z} \right) \]

\[ = e^{ikD} \int_{r=0}^{\infty} e^{\frac{i\pi}{\lambda z} (x_0^2 + y_0^2)} e^{i\phi} D e^{-i\pi \lambda \left(\frac{1}{D} + \frac{1}{z}\right)} \frac{i\lambda}{D} + \frac{1}{z} \]

\[ = e^{ik(D+z)} D e^{i\pi \left[\frac{1}{2} (x^2 + y^2) - \left(\frac{1}{D} + \frac{1}{z}\right) (x_0^2 + y_0^2)\right]} \] (8.48)

This can be recognized as the parabolic wavefront approximation to a spherical wave on a screen, illustrating the consistency of the Fresnel integral in this approximation.

**8.3.1 One dimensional mask approximation**

The critical assumption is that the amplitude function \( f(x, y, 0) \) can be modelled as a product of the incident spherical wave and a transmission mask function \( \tilde{q}(x, y) \) (note transmission function is now denoted by \( \tilde{q} \) instead of \( q \) to avoid confusion with the spatial frequency \( q \)). Furthermore if the mask is separable and can be written as a function of \( x \) alone, then amplitude function at the object plane can be written as the product of the spherical wave \( f_0(x, y, 0) \), emitted from the source and the transmission function \( \tilde{q}(x, y, 0) \) at the object plane as

\[ f(x, y, 0) = \tilde{q}(x, y, 0) f_0(x, y, 0) \approx \tilde{q}(x) f_0(x, y, 0) \] (8.49)
Then the general Fourier term, Eq. 8.40 becomes

$$F(p, q) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y, 0)e^{i \frac{\pi}{\lambda z}(x^2+y^2)}e^{-i2\pi(px+qy)}dxdy$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{q}(x)f_0(x, y, 0)e^{i \frac{\pi}{\lambda z}(x^2+y^2)}e^{-i2\pi(px+qy)}dxdy$$  (8.50)

which is now separable, and using the spherical wave emitted by the source Eq. 8.41, this can now be written as

$$F(p, q) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{q}(x)e^{ikD}e^{\frac{ikD}{\lambda z}(x^2+y^2)}e^{i\pi x^2 \lambda} \left[ 1 + \frac{1}{\lambda D} \right]^{-i2\pi px} dx \int_{-\infty}^{\infty} e^{i\pi y^2 \lambda} \left[ 1 + \frac{1}{\lambda D} \right]^{-i2\pi qy} dy$$  (8.51)

Here the fibre modulates the integral over $x$, while the integral over $y$ is a scaling factor. It is possible to determine the scaling factor by first postulating that if the transmission function were $\tilde{q}(x) = 1$, then Eq. 8.51 would be

$$F_0(p, q) = \frac{e^{ikD}}{D} \int_{-\infty}^{\infty} 1 \cdot e^{i\pi x^2 \left[ \frac{1}{\lambda D} + \frac{1}{z} \right]} e^{-i2\pi px} dx \int_{-\infty}^{\infty} e^{i\pi y^2 \left[ \frac{1}{\lambda D} + \frac{1}{z} \right]} e^{-i2\pi qy} dy$$

$$= \frac{e^{ikD}}{D} F_1(p) F_1(q)$$  (8.52)

Comparing Eq. 8.52 with the previously calculated polar form, Eq. 8.47

$$F_0(p, q) = \frac{e^{ikD}}{D} e^{-\frac{ix}{\lambda \left( \frac{1}{\lambda D} + \frac{1}{z} \right)}(x_0^2+y_0^2)} i\lambda \left( \frac{1}{\lambda D} + \frac{1}{z} \right)$$

$$= \frac{i\lambda}{D \left( \frac{1}{\lambda D} + \frac{1}{z} \right)} e^{ikD} e^{-\frac{ix}{\lambda \left( \frac{1}{\lambda D} + \frac{1}{z} \right)}(x_0^2+y_0^2)} e^{-i\pi \left( \frac{1}{\lambda D} + \frac{1}{z} \right)y_0^2}$$  (8.53)
The parts $F_1(p)$ and $F_1(q)$ may now be determined

$$F_1(p) = \sqrt{\frac{i\lambda}{(\frac{D}{2} + \frac{z}{2})}} e^{-\frac{i\pi}{\lambda} (\frac{D}{2} + \frac{z}{2}) y_0^2}$$

$$F_1(p) = e^{i\frac{\pi}{4}} \sqrt{\frac{\lambda D z}{(D + z)}} e^{-i\pi \left\{ \frac{\lambda D z}{(D + z)} \right\} y_0^2}$$

(8.54)

$$F_1(q) = e^{i\frac{\pi}{4}} \sqrt{\frac{\lambda D z}{(D + z)}} e^{-i\pi \left\{ \frac{\lambda D z}{(D + z)} \right\} y_0^2}$$

substitute for $y_0$

$$F_1(q) = e^{i\frac{\pi}{4}} \sqrt{\frac{\lambda D z}{(D + z)}} e^{-i\pi \left\{ \frac{\lambda D z}{(D + z)} \right\} q^2}$$

(8.55)

where Eq. 8.43 has been used in substituting for $y_0$. Now the Fourier equation, Eq.8.51 becomes

$$F(p, q) = \frac{e^{ikD}}{D} \sqrt{\frac{\lambda D z}{(D + z)}} e^{-i\pi \left\{ \frac{\lambda D z}{(D + z)} \right\} y_0^2} \int_{-\infty}^{\infty} q(x) e^{i\frac{\pi}{\lambda} \left\{ \frac{D x^2}{2} + \frac{1}{2} \right\} - i2\pi p x} dx$$

(8.56)

However, the integral over plus to minus infinity is not practical, hence as before (with Fresnel-Kirchhoff diffraction), use is made of Babinet’s type formulation

$$\int_{-\infty}^{\infty} q(x) e^{\psi(x)} dx = \int_{-\infty}^{-a'} e^{\psi(x)} dx + \int_{-a'}^{a} q(x) e^{\psi(x)} dx + \int_{a}^{\infty} e^{\psi(x)} dx$$

(8.57)

As before (Section 8.1.5) the term $\int_{-a'}^{a} e^{\psi(x)} dx$ is added and subtracted away again.

$$\int_{-\infty}^{\infty} q(x) e^{\psi(x)} dx = \int_{-\infty}^{-a'} e^{\psi(x)} dx + \int_{-a'}^{a} e^{\psi(x)} dx + \int_{-a'}^{a} q(x) e^{\psi(x)} dx + \int_{-a'}^{a} e^{\psi(x)} dx + \int_{a}^{\infty} e^{\psi(x)} dx$$

$$i + ii + iii = \text{same as no fibre}$$

(8.58)
Therefore the Fourier equation, Eq. 8.56 becomes

\[ F(p, q) = F_0(p, q) + \frac{e^{ikD}}{D} \sqrt{\frac{\lambda Dz}{D + z}} e^{-i\pi \left(\frac{\lambda Dz}{D + z}\right)q^2} e^{i\frac{z}{z}} \int_{-a'}^{a'} \tilde{q}(x) - 1 \right] e^{i\pi z^2 \left(\frac{1}{D} + \frac{1}{z}\right) - i2\pi px} \, dx \]

Substituting this into Eq. 8.39

\[ f(x, y, z) = \Gamma \left\{ F_0(p, q) + \frac{e^{ikD}}{D} \sqrt{\frac{\lambda Dz}{D + z}} e^{-i\pi \left(\frac{\lambda Dz}{D + z}\right)q^2} e^{i\frac{z}{z}} \int_{-a'}^{a'} \tilde{q}(x) - 1 \right] e^{i\pi z^2 \left(\frac{1}{D} + \frac{1}{z}\right) - i2\pi px} \, dx \right\} \]

where

\[ \Gamma = \frac{e^{ikz}}{i\lambda z} e^{\frac{z}{D}(x^2 + y^2)} \quad (8.59) \]

Using Eq. 8.47 repeated here

\[ F_0(p, q) = \frac{e^{ikD}}{D} e^{i\pi \left(\frac{1}{D} + \frac{1}{z}\right)(x_0^2 + y_0^2)} \frac{i\lambda}{\left(\frac{1}{D} + \frac{1}{z}\right)} \]

\[ = \frac{i\lambda e^{ikD}}{D + z} e^{-i\pi \left(\frac{1}{D} + \frac{1}{z}\right)(x_0^2 + y_0^2)} \quad (8.60) \]

The transform variables \(x_0\) and \(y_0\) may be written

\[ x_0 = \frac{\lambda p}{D + z} = \frac{\lambda p Dz}{D + z} \]

and \( p = \frac{\lambda x}{\lambda z} \)

\[ \therefore x_0 = \frac{\lambda x Dz}{D + z} = \frac{x D}{D + z} \]

Similarly \( y_0 = \frac{y D}{D + z} \quad (8.61) \)
Thus the Fourier term without the fibre, Eq. 8.60 may be written

\[
F_0(p, q) = i\lambda z e^{ikD} \frac{e^{-i\pi [\frac{D}{D^2} + \frac{z}{D^2}]}}{D + z} = i\lambda z e^{ikD} \frac{e^{-i\pi [\frac{D}{D^2} + \frac{z}{D^2}]}}{D + z} \left( x^2 + y^2 \right) \]

(8.62)

Then Eq. 8.59 becomes,

\[
f(x, y, z) = \Gamma \left\{ 1 + \sqrt{\frac{D + z}{\lambda D z}} e^{i\pi \frac{D}{\lambda D z}} \sqrt{\frac{\lambda D}{\lambda D z}} e^{-i\pi [\frac{D}{D^2} + \frac{z}{D^2}]} e^{i\pi \frac{x}{\lambda D z}} \int_{-a'}^{a'} [\tilde{q}(x) - 1] e^{i\pi \frac{x^2}{\lambda D z}} [\frac{1}{\frac{D}{D^2} + \frac{z}{D^2}} - i2\pi px] dx \right\}
\]

(8.63)

where

\[
\Gamma = \frac{e^{ikz}}{i\lambda z} e^{i\pi \frac{x}{\lambda D z}} (x^2 + y^2) \frac{i\lambda z e^{ikD} e^{-i\pi [\frac{D}{D^2} + \frac{z}{D^2}]} \Gamma}{D + z} = \frac{e^{ik[(D + z)](D + z)}}{D + z} e^{i\pi \frac{x}{\lambda D z}} \left( x^2 + y^2 \right) \frac{1}{\frac{D}{D^2} + \frac{z}{D^2}}
\]

(8.64)

The final form is

\[
f(x, y, z) = \Gamma \left\{ 1 + \sqrt{\frac{D + z}{\lambda D z}} e^{i\pi \frac{x}{\lambda D z}} (x^2 + y^2) \int_{-a'}^{a'} [\tilde{q}(x) - 1] e^{i\pi \frac{x^2}{\lambda D z}} [\frac{1}{\frac{D}{D^2} + \frac{z}{D^2}} - i2\pi px] dx \right\}
\]

(8.65)

which is used in the simulation programs.
8.3.2 Resulting diffraction patterns

The resulting diffraction patterns are now similar to experiment and more satisfactory than the Fresnel-Kirchhoff diffraction patterns. An un-normalized single energy (10 keV) with geometry $r_s = 0.05 \, \text{m}$ and $r_d = 1.95 \, \text{m}$, example is shown in Fig. 8.21 which compares favourably to an experimentally equivalent line profile in Fig. 8.22. The characteristic ‘double peaks’ of the fibre edges from experiment are also present in the simulations with added structure in the negative peaks. There is a difference in absolute value of the intensity patterns but this is a very difficult area to match and relative shapes are considered sufficient at this stage.

To see how the resulting diffraction patterns for the measured spectrums are constructed, the line profiles of the raw Fresnel diffraction calculations for just the left side of fibre profile for selected energies are shown in Fig. 8.23. It can be noticed...
that although the magnitudes and patterns vary for each energy, there is a region of similarity corresponding to the edges of the fibre, which add constructively while the differences add destructively to form the background.

If these patterns are weighted and summed together according to a measured spectrum say for example an unfiltered spectrum, see Fig. 8.24, which has a large bremsstrahlung component with three L characteristic peaks, then the resultant diffraction pattern is constructed as shown in Fig. 8.25. This produces a phase contrast of $\gamma = 0.86$, which is about a factor of 4 greater than the experiment.

It is worthwhile to determine the relative contributions to the diffraction pattern from the various parts of the spectrum, as for example the large L peaks may be the dominant contribution. The contributions to the diffraction pattern are shown in Fig. 8.26. It shows that the three L lines, are the dominant contributions per energy.
CHAPTER 8. DIFFRACTION SIMULATIONS

Figure 8.23: Raw Fresnel diffraction for selected energies

Figure 8.24: Experimental measurement of unfiltered spectrum
of the diffraction pattern in proportion to their relative strengths which is the natural assumption. The effect of a cumulative sum of the energy contributions is shown in Fig. 8.27, which shows the relative proportions of each energy range. It is interesting to note that although the $L$ peaks contribute significantly to the overall diffraction pattern, there is an equally large contribution from the high energy ‘tail’, i.e. 12 to 30 keV. Even though the contribution from each energy in this regime is small, due to the large range, they sum to a significant proportion. Furthermore, the higher energy photons contribute more to the overall diffraction intensity pattern than lower energy photons. This finding was contrary to an initial hypothesis that the characteristic $L$ lines were mainly responsible for the resulting diffraction pattern or lack of them for the filtered case. The relative contributions for a 0.94 mm Al filtered spectrum (Fig. 8.28) are shown in Fig. 8.29, where it can be seen that the dominant contributions are from the higher energies. Colours corresponding to the energy regimes are shown
CHAPTER 8. DIFFRACTION SIMULATIONS

Figure 8.26: Contributions from energy regimes for unfiltered spectrum

Figure 8.27: Cumulative sum of Fresnel patterns for selected energy regimes
CHAPTER 8. DIFFRACTION SIMULATIONS

Figure 8.28: Measured filtered spectrum for 0.94mm Aluminium at 30 keV tube potential

Figure 8.29: Cumulative sum of filtered Fresnel patterns for the same energy regimes, showing dominant contributions from higher energies

in Fig. 8.28, where it can be seen that the spectrum is shifted up towards the higher energies as the lower ones are filtered out. The resulting Fresnel diffraction pattern is shown in Fig. 8.30, which shows little difference to the unfiltered pattern with a phase contrast of $\gamma_f = 0.78$

In this case the difference in phase contrast is very minor and for some geometries is actually greater than the unfiltered spectrums, showing that the spectrum change alone is not the cause of phase contrast loss.
Figure 8.30: Filtered raw Fresnel diffraction pattern for fibre, $r_s=0.05$ m, $r_d=1.95$ m, 30 kVp, 0.94 mm Al

No assumptions have been made for efficiency of the detector at this stage which is addressed in the next section.

8.4 Detector and Source considerations

8.4.1 Image plate detection efficiency

To account for the detector efficiency and the incident power density in a more complete way, use is made of a semi-empirical model as described by Tucker and Rezentes [181]. There are two factors to consider, the power spectral density of x-rays incident upon the image plate, and the detection efficiency of the plate. The power spectral density is given by

$$P(E, x) = E N(E) |f(x, 0, z)|^2$$  \hspace{1cm} (8.66)

where $E = hc/\lambda$ is the incident energy of the x-rays, $N(E)$ is the measured photon flux distribution. The area density of the energy deposited on the Photostimulable
Phosphor (PSP) of the image plate is proportional to

\[ E_p(x) = \int_0^\infty y(E) P(E, x) \, dE \]  \hspace{1cm} (8.67)

where \( y(E) \) is the energy absorption efficiency of the PSP. A plot of efficiency versus energy is shown in Fig. 8.31. A comparison of the simple model without detector efficiency correction and the semi-empirical model is shown in Fig. 8.32. As can be seen there is a little change to the peaks in the resulting diffraction pattern, increasing the outer peak and decreasing the inner one.

8.4.2 Image plate scanning convolution

The image plate scanner uses a laser with a finite size to determine the recorded x-ray exposure as a quantized pixel value. This can be modelled as a convolution of \( E_p(x) \)
with a Gaussian profile with a standard deviation, \( \sigma \) equal to the corresponding full width, half maximum (FWHM) of the laser beam at 25 µm, which is about 15 µm.

\[
\omega_{\text{detector}} = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{1}{2}(\tilde{x})^2}
\]  

(8.68)

The shape of the detector convolution profile is shown in Fig. 8.33. The detector convolution profile is fairly narrow and remains constant unless the scanner settings are changed to 50 µm resolution.

### 8.4.3 Source size convolution

Assuming there is zero transverse coherence length between source points, the simplest geometrical configuration of a circular source is used [182]. Referring to Fig. 8.34
Figure 8.33: Detector convolution profile as a function of distance across the image plane

Figure 8.34: Schematic of circular source with radius $s_r$. 
Consider an elemental source area \(dxdy\), which produces an elemental intensity \(d\hat{I}\), as a fraction of the entire emitting area that has a radius \(s_r\).

\[
d\hat{I} = \frac{dxdy}{\pi s_r^2}
\]  

(8.69)

If this elemental area is integrated over say the y direction, and produces a function \(\ell(x)\) then the elemental strip \(dI\) is

\[
dI = \frac{\ell(x)dx}{\pi s_r^2} = \frac{\sqrt{s_r^2 - x^2} \, dx}{\pi s_r^2}
\]  

(8.70)

where \(\ell(x)\) is assumed to vary as a semicircular type function

\[
\ell(x) = \sqrt{s_r^2 - x^2}
\]  

(8.71)

The effect of the extended source, as shown in Fig. 8.35, is to shift the fibre diffraction pattern, \(f(x, y)\), to \(f(x - \frac{x'}{D}, y - \frac{y'}{D})\), according to the position of the
elemental source. The total effect is found by summation over the entire source area.

\[
I(x, y) = \int \int f(x - \frac{zx'}{D}, y - \frac{zy'}{D}) \frac{dx'dy'}{\pi s_r^2} I_s(x', y')
\]

\[
= \int dx' \int dy' I(x', y') \frac{I(x', y')}{\pi s_r^2} f(x - \frac{zx'}{D})
\]

change of variables \( x'' = \frac{zx'}{D} \)

\[
= \frac{D}{z} \int dx'' \omega_s(x'') f(x - x'') \quad (8.72)
\]

and this can be recognized as convolution of the source function \( \omega_s \) with the diffraction pattern \( f(x, y) \). The source function \( \omega_s \) can be written as

\[
\omega_s(x') = \frac{\sqrt{s_r^2 - x'^2}}{\pi s_r^2} \quad (8.73)
\]

and with the change of variables this becomes

\[
\frac{D}{z} \omega_s\left(\frac{Dx''}{z}\right) = \frac{D\sqrt{s_r^2 - \left(\frac{Dx''}{z}\right)^2}}{z \pi s_r^2}
\]

\[
= \frac{\sqrt{\frac{s_r^2}{z^2} - (Dx'')^2}}{(\frac{z}{D})^2 \pi s_r^2}
\]

\[
= \frac{\sqrt{\rho^2 - (x'')^2}}{\pi \rho^2}
\]

where \( \rho = \frac{z r_s}{D} \) \quad (8.75)

A profile of the source convolution is shown in Fig. 8.36. The greater magnitude of the source convolution profile compared to the detector convolution (see Fig. 8.33) reflects the greater influence of the source on the final diffraction pattern for this particular geometry.
8.4.4 Total convolution

The final diffraction pattern is obtained by convolving the Fresnel patterns after corrections for detector efficiency, with the above detector and source profiles. The two convolutions can be combined into

\[ \omega(x) = \omega_s \ast \omega_{\text{detector}}(x) \]  

(8.76)

For geometries of \( r_s = 0.05 \text{ m} \) and \( r_d = 1.95 \text{ m} \) with source size of 4 microns diameter, the results of the total and component convolutions are shown in Fig. 8.37. In this case the source convolution is the major factor in the reduction of phase contrast.

8.4.5 Phase contrast as a function of kVp

Variation of phase contrast with tube potential (kVp) can be seen in Fig. 8.38. There is a steady decrease of phase contrast with an increase of kVp except for the 80 kVp value which is most likely an error. This is due to the range limitations of SiLi detector which is unable to measure beyond 60 kVp accurately, and hence the spectra for used for 70 and 80 kVp are not accurate for use in the simulation calculation for phase
Figure 8.37: Total and component convolutions for $r_s=0.05\text{m}$, $r_d=1.95\text{m}$ for unfiltered case (30 kVp), for $4\mu\text{m}$ source and $25\mu\text{m}$ scanning laser beam

contrast.

Compared to the measured values of phase contrast with kVp, chapter 6 (Fig. 6.6), these calculated values are about a factor 3 to 4 bigger and some reasons for this discrepancy are discussed in the next section.

### 8.4.6 Phase contrast as a function of source size

The question of how phase contrast varies with source size is now considered. As source increases, it is expected that it would dominate the total effect while the detector effect would remain constant. The calculated phase contrast as a function of source size can be seen in Fig. 8.39 where the individual contributions to the total phase contrast are
shown. The calculated phase contrast values are much higher than the ones measured in chapter 6, and displayed in Fig. 6.3. For example, the calculated phase contrast at 4 µm source size, with the same parameters as the experiment, is $\gamma_{\text{cal}} \simeq 0.55$, compared to the experimental equivalent $\gamma_{\text{exp}} \simeq 0.22$.

Since phase contrast is highly sensitive to the source size, there was a hope to explain the discrepancy of experiment and simulated phase contrast values as a result of the source size error since the simulated ones were too high. It is known that the source is not circular and at least larger in the horizontal direction than the vertical (see Gureyev [183]). Hence by increasing the source size in the convolution calculation there was a hope that a small increase to say 5 or 6 µm might find a better match to experiment. However this is not the case as the source size would have to increase dramatically from the 4 µm nominal size to about 10 µm. Hence there may be other
8.4.7 Phase contrast as a function of source to object distance

It is known from experiment that phase contrast changes as a function of source to object distance (chapter 6, Fig. 6.9). This change is also reflected in the simulations, as shown in Fig. 8.40, performed at 30 kVp, with an unfiltered x-ray spectrum and for the moment, without system effects. The line profiles can be seen to move systematically towards the zero mark, or center of the detector on the right hand side of the graphs, as the magnification is decreased. The last subplot of the figure is a plot of phase contrast versus distance $r_s$ ($r_s = R_1$ in the figure). The variation with distance without source
and detector considerations has only a faint resemblance to the experimental case. However, when the various contributions from the source and detector are included, as

![Image of Fresnel patterns](image)

**Figure 8.40:** Raw diffraction Fresnel patterns for various distances of object to source. Note the patterns moving closer to the zero mark on the right hand side and that \( R_1 \equiv r_s \)

shown in Fig. 8.41 and Fig. 8.42, initially for \( r_s = 0.05 \) m, the source dominates the total result until around \( r_s = 0.3 \) m, where the detector convolution swaps as the dominant effect.

Tabulated values of the various contributions are given in Table 8.1, where for the distance \( r_s \), the calculated phase contrast for the source alone, detector alone and total
Figure 8.41: Variation of diffraction pattern with object to source distance for $0.05 \leq r_s \leq 0.76$. Note $R_1 = r_s$ in the figure.

These values can be seen more clearly for comparison in Fig. 8.43, where the effects of source convolution reduce with increasing $r_s$, while the detector convolution increases its influence. The source convolution dominates from $0 < r_s \leq 0.3$ m, but the detector convolution dominates afterwards, with the maximum phase contrast occurring for $r_s = 0.3$ m, and the total phase contrast reducing with the detector convolution from $0.3 \leq r_s \leq 1.6$ m. A more interesting comparison is with the experimental data, as shown in Fig. 8.44. Although the scaling is different which may be due to a number of factors, the general shape of the relationship is consistent with experiment, as can be
Figure 8.42: Variation of diffraction pattern with object to source distance for $0.89 \leq r_s \leq 1.53$. Note $R_1 = r_s$ in the figure

<table>
<thead>
<tr>
<th>$r_s$ in meters</th>
<th>Source</th>
<th>Detector</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>0.56973</td>
<td>0.80516</td>
<td>0.553</td>
</tr>
<tr>
<td>0.26</td>
<td>0.87819</td>
<td>0.78995</td>
<td>0.75196</td>
</tr>
<tr>
<td>0.47</td>
<td>0.92506</td>
<td>0.72037</td>
<td>0.7063</td>
</tr>
<tr>
<td>0.68</td>
<td>0.94445</td>
<td>0.61308</td>
<td>0.6072</td>
</tr>
<tr>
<td>0.89</td>
<td>0.95163</td>
<td>0.49523</td>
<td>0.49238</td>
</tr>
<tr>
<td>1.11</td>
<td>0.95476</td>
<td>0.3823</td>
<td>0.38128</td>
</tr>
<tr>
<td>1.32</td>
<td>0.95285</td>
<td>0.27941</td>
<td>0.2791</td>
</tr>
<tr>
<td>1.53</td>
<td>0.93309</td>
<td>0.1861</td>
<td>0.18598</td>
</tr>
</tbody>
</table>

Table 8.1: Table of calculated phase contrast values as a function of source to object distance (30 kVp unfiltered spectrum)
Figure 8.43: Calculated phase contrast comparisons of source, detector and total convolutions
further seen when a scaling factor is introduced to make them comparable as shown in Fig. 8.45. There is a slight mismatch, in the positions indicating some systematic positioning error.

8.4.8 Phase contrast as a function of different materials

The effect of various materials as filters is shown in Fig. 8.46. There is a strong reduction in phase contrast with material thickness and increasing Z. Silicon which has atomic number 14 has almost identical effect on phase contrast as aluminium (Z=13). Copper (Z=29) and nickel (Z=28) have nearly identical effect on phase contrast, while PMMA, which is mostly carbon (Z=6) has the least effect. Interestingly the placement of the filter as in the case of aluminium near the detector has minimal effect, as does the grain size of aluminium.

For comparison for the case of aluminium filters, theory and experiment are shown on the same graph in Fig. 8.47. Although the absolute values between theory and experiment are different, there is some variability of the theoretical predictions regarding source and detector sizes. Although the scanner setting was 50 µm, this is not the intrinsic resolution of the detector system, due to the granularity in the screen structure which scatters the stimulating laser light [184]. Therefore the phase contrast values had been recalculated for two higher effective resolutions of 160 and 200 µm, which consequently shows a reduction in theoretical phase contrast values, closer to that of experiment. This will be discussed more fully in the discussion chapter.

8.4.9 Summary

This chapter has modelled the phase contrast process on the Fresnel diffraction formulism which matches the experiment reasonably well except for an absolute difference of about 2, if the detector resolution is allowed to increase significantly
Figure 8.44: Simulation comparison with experiment for phase contrast versus source to object distance
Figure 8.45: Simulation comparison with experiment with scaling for phase contrast versus source to object distance
Figure 8.46: Expanded view of calculated phase contrast as a function of different filter materials and thicknesses

to around 150-160 µm. It also matches the line profiles obtained through the ray tracing method which gives confidence that the simulation is correctly modelling the experiment. The effect of materials in filtering the incident beam is to narrow the diffraction peaks, which by itself does not change the phase contrast index of the line profiles very much. This narrowing is due to the reduced dispersion in the fibre of the hardened spectra. It is only when the source and detector convolutions are considered, that the filters change the line profiles dramatically, effectively reducing phase contrast index with spectral hardness.
Figure 8.47: Experimental phase contrast as a function of filter thickness, obtained at 30 kVp, 100 μA, \( r_s=55 \text{ cm}, \ r_d=145 \text{ cm}, \) 50 μm detector setting, plus scaled experimental to maximum phase contrast value. Theoretical predictions for 4 μm source size, with 25, 160 and 200 μm detector resolution.
Chapter 9

Discussion

Although the simulation describes the main features of phase contrast reduction with filters, the simulated absolute values remain much higher than the experimental ones. Some factors which may have impacted on these figures are explored.

While noise was not included into the simulation and may be a worthwhile activity, there are other mechanisms which are likely to be more dominant. The most notable is the detector resolution, which if increased to 160 $\mu$m and greater, gives a predicted phase contrast closer to that of experiment. The striations or surface roughness of the fibre has been taken into account somewhat by the fibre straightening algorithm which improved the consistency of phase contrast measurements but at the expense of phase contrast peak. Including noise into the simulation may lower the phase contrast prediction but not to the extent required to match theory.

Some quantification of this is as follows. The phase contrast metric $\gamma$ used in thesis is defined in Eq. 6.4 given here again as

$$\gamma = \frac{(a - b)}{(a + b)} - \frac{(a' - b')}{(a' + b')}$$

(9.1)
where \( a \) = the positive peak maximum, \( b \) = the negative peak minimum, \( a' \) = the absorption outside the object and \( b' \) = the absorption inside the object.

The variance and hence standard deviation is given by Eq. 6.5 reproduced here

\[
\text{Var}(\gamma) \approx \left( \frac{\partial \gamma}{\partial a} \right)^2 \text{Var}(a) + \left( \frac{\partial \gamma}{\partial b} \right)^2 \text{Var}(b) + \left( \frac{\partial \gamma}{\partial a'} \right)^2 \text{Var}(a') + \left( \frac{\partial \gamma}{\partial b'} \right)^2 \text{Var}(b')
\]

\[
\sigma_\gamma^2 = \frac{4b^2}{(a + b)^4} \sigma_a^2 + \frac{4a^2}{(a + b)^4} \sigma_b^2 + \frac{4b'^2}{(a' + b')^4} \sigma_{a'}^2 + \frac{4a'^2}{(a' + b')^4} \sigma_{b'}^2
\]

\[
\leq \frac{4}{(a + b)^4} (b^2 + a^2) \sigma_a^2 + \frac{4}{(a' + b')^4} (b'^2 + a'^2) \sigma_{a'}^2
\]

In this case, it is the standard error that is required, therefore the variance must be divided by the sample size \( N \). Therefore the error in phase contrast is \( \frac{\sigma_\gamma}{\sqrt{N}} \) and the phase contrast is given by

\[
\gamma = \bar{\gamma} \pm \frac{\sigma_\gamma}{\sqrt{N}} \quad (9.2)
\]
An image of a fibre taken at 30 kVp, 100 µA, $r_1 = 14$ mm at 50 µm is shown in Fig. 9.2. The two edges of the fibre can be clearly seen. Taking the mean over 512 rows gives the line profile as shown in Fig. 9.3. The row mean is shown in context with individual line profiles in Fig. 9.4. The line profile of the mean can be seen against the noisy individual profiles in the background, together with standard deviation at the lower portion of the graph. For the left-hand edge, the mean positive peak value is $a = 3396$ and the standard error $e_a = 9$. The mean negative peak is $b = 2784$ with $e_b = 8$. Outside of the fibre towards the left, the mean absorption value is $a' = 3182$ with $e_{a'} = 3$, while on the inside, $b' = 3181$ with $e_{b'} = 3$. The phase contrast value is $\gamma = 0.099$ with $e_\gamma = 0.002$.

The largest contributing factor to the phase contrast error is $e_a$. To see the effect on the phase contrast error, $e_a$ was allowed to vary from 0 to 450 and $e_\gamma$ calculated via Eq. 9.2 and plotted in Fig. 9.5. The current error in the peak height value is shown as $(9,0.002)$, which means $e_a \approx 9$ which results in $e_\gamma \approx 0.002$. To give an error
Figure 9.3: Mean line profile showing data points for row averaging (blue) and line for column averaging (green) for 50 µm scan

Figure 9.4: Mean line profile against individual row profiles showing the variation in psl brightness for 50 µm scan
Figure 9.5: Phase contrast psl error $e_\gamma$ versus error in peak height $e_a$ for 50 $\mu$m scan

comparable to the mean phase contrast value (to give a possible doubling mechanism of phase contrast) $\gamma \simeq 0.09$, the corresponding error can be seen to be $\sigma_a \gg 450$ which is nearly a fifty-fold increase in the standard error for $e_a$. This is clearly not the case, therefore the effect of noise in measuring experimental phase contrast is not responsible for the mismatch between theory and experiment.

The same fibre imaged under the same conditions but scanned at 25 $\mu$m is shown in Fig. 9.6. More data points can be seen around the positive and negative phase peaks for 25 $\mu$m scan in Fig. 9.7. The column mean line profile is not shown as it is not the same length as the row mean. To observe the row mean in context with the noisy individual line profiles see Fig. 9.8. The standard deviation and standard deviation plus an offset are also shown. The standard deviation for both positive and negative phase peaks is reduced compared to the 50 $\mu$m scan.

In this case $a = 3059$ with $e_a = 8$, $b = 2415$ with $e_b = 7$, outside the fibre the mean value is $a' = 2818$ with $e_{a'} = 0.4$, while on the inside, $b' = 2813$ with $e_{b'} = 0.4$. The
Figure 9.6: X-ray image of a fibre taken at 30 kVp, 100 µA, \( r_1 = 14 \) mm at 25 µm with a straight edge for comparison

Figure 9.7: Mean line profile showing data points for row averaging (cyan) for 25 µm scan
Figure 9.8: Mean line profile against individual row profiles showing the variation in psl brightness for 25 µm scan

phase contrast value is $\gamma = 0.12$ with $e_\gamma = 0.0018$. The current error in the peak height value is shown as $(8,0.002)$, which means $e_a \simeq 8$ which results in $e_\gamma \simeq 0.002$. To give an error comparable to the mean phase contrast value $\gamma \simeq 0.117$, the corresponding error by the graph can be seen to be $e_a \gg 450$ which is nearly a sixty-fold increase in the standard error for this value. This is clearly not the case, therefore noise in measuring experimental phase contrast is not responsible for the mismatch between theory and experiment.

Exploring the effect of the density of the fibre (cellulose) on phase contrast, by reducing it from 2000 kg/m$^3$ down to 20 ie 1/100th of its previous value, Fig. 9.1 shows the relationship to phase contrast with density. The results show a reduction in phase contrast as the density decreases showing numerical values similar to experiment when density is about 500 rather than 2000 kg/m$^3$. However, it is not enough to explain the discrepancy.
Figure 9.9: Phase contrast psl error $e_\gamma$ versus error in peak height $e_a$ for 25 $\mu$m scan

Figure 9.10: Fresnel diffraction patterns for fibre edge with various detector resolutions at FWHM i.e $\sigma$
The image plate detector resolution at 25 µm however, is not the resolution of the system as this is only the scanner resolution, as subsequent light scatter within the active material of the image plate increases this to an effective resolution somewhere between 80 to 200 microns, depending on the system and type of image plate. Therefore Fig. 9.10 shows how this would effect the line profile patterns. The calculated phase contrast values for the unfiltered case at $r_s=0.055$ m are shown in Fig. 9.11 as a function of the parameter FWHM. Since the phase contrast values for the experimental data without added filtration, is around 0.12, this would require the detector to have a resolution of about 150 microns, if this were the sole effect. This could be the subject of future work.

Another possibility is the source focus. It was known from previous work in this thesis, that observations of optimal phase contrast values between 0.2-0.25 were noted for the case of unfiltered beam for an $r_s$ distance of around 20 cm, which may mean that
the source was not properly focussed at 4 \( \mu m \). Therefore the source focus and/or shape could have been a variable affecting the experimental phase contrast index. Perhaps this should have been established at each set of imaging experiments using the gold mask test object with a measurement of observed line pair patterns. However this is a very tedious business and one would hope that it would not be necessary to do so frequently.

For a microfocus tube there is not much correlation between emission points since the electrons in the beam have no correlation and the distance to the fibre from the source is small. Hence the individual elements of the source have been modelled as incoherent and completely independent. This contrasts with synchrotrons where the electrons have some degree of correlation and the distances from the source to object are so great that there may indeed be correlation across the object. Thus the effects of partial coherence have been deliberately omitted in the simulations conducted and the finite source size has been incorporated as a blurring convolution which is common practice with a micro-focus type anode source [185], [186].

An interesting note as pointed out by Wu and Lui [187], about coherence, particularly lateral coherence \( L_\perp \) which is the transverse distance over which the wavefield is strongly correlated, typically defined as

\[
L_\perp = \frac{\bar{\lambda} r_s}{s}
\]  

(9.3)

where \( r_s \) is the source to object distance, \( s \) is the finite source size and \( \bar{\lambda} \) is the wavelength, is that although this equation is derived for a narrow band of wavelength, from the mutual intensity function of quasimonochromatic waves, it holds also for polychromatic waves as the cross-spectral density functions also obey the same laws. They point out the confusion in the literature about the requirement of \( L_\perp \) for phase-contrast visibility, which at a distance of \( r_s = 1 \text{ m} \), source size of 10 \( \mu \text{m} \) and wavelength \( \lambda=1.24\AA \), \( L_T \) is only 0.124 \( \mu \text{m} \). To obtain say a lateral coherence, \( L_T \) of 50 \( \mu \text{m} \) as required in clinical practice, the source to object distance \( r_s \) would have to be around
4 m which is not very practical. They propose an alternative definition based on a phase space approach and Wigner distributions which is different to the usual paraxial Fresnel diffraction formalism covered here. The interested reader is directed to their papers [113] and [85]. They define the quantity $L_{\text{shear}}$ as a phase-space shearing which leads to a wave superposition for forming phase-contrast,

$$L_{\text{shear}} = \frac{\lambda r_d}{M}$$

(9.4)

where $r_d$ is the object to detector distance, and $M$ is the magnification. When this is divided by the lateral coherence length $L_T$, it becomes the quantity that determines the coherence effects on the phase-contrast visibility of an object

$$\frac{L_{\text{shear}}}{L_T} = \frac{r_d s |u|}{M r_s} = \frac{(M - 1)s |u|}{M}$$

(9.5)

where $u$ is a spatial frequency of the object and noting that this equation is wavelength independent. Thus for a given spatial frequency $u$, if $\frac{L_{\text{shear}}}{L_T} \ll 1$ produces nearly full coherence while $\frac{L_{\text{shear}}}{L_T} \gg 1$ produces no coherence and correspondingly there is no phase contrast. Thus for example for distances $r_s = 0.2$ m, $r_d = 1.8$ m, a spatial frequency of $|u| = 1/50$ µm and source size, $s = 10$ µm, the phase space shearing $\frac{L_{\text{shear}}}{L_T} = 0.16$, which is less than one and hence the arrangement produces moderate coherence and phase-contrast visibility.
Chapter 10

Conclusion

Although the absolute theoretical phase contrast values are higher than the experimental ones, there is a consistent trend that allows some conclusions to be drawn. It is known that phase contrast decreases with an increase in tube voltage, source size and filter thickness, and also that it has a complicated relationship with the imaging geometry [185]. The calculated theoretical values, based on the Fresnel diffraction, followed the same trends in each case. In the case of reduction of phase contrast by added filters, the ultimate conclusion is that it is due to beam hardening caused by the bulk material of the filter. However, this is only because of system limitations and is not due to inherent decrease of phase contrast by beam filtration. The filter causes the spectrum to shift to higher energies, as measured by the SiLi detector. The higher energies produce a narrowing of the diffraction peaks that give phase contrast, but does not reduce their amplitude. The system function smooths and reduces these narrower peaks. Thus if a better system could be designed with finer detector resolution, and smaller source size, then the phase contrast loss would not be so dramatic. Furthermore, the phase contrast loss is not due to surface properties or grain structure of the filters, hence conventional filters may be used for the polychromatic spectrum of the micro-focus type tubes.
Nesterets et al [185], derive equations for optimal phase contrast for certain parameters such as contrast, signal to noise ratio (SNR), resolution and sampling including the optimal geometrical magnification $M = (r_s + r_d)/r_s$, based on $\sigma_s$ and $\sigma_d$ that characterize the source and detector resolution and give the relationship

$$M_{opt} = 1 + \left( \frac{\sigma_d}{\sigma_s} \right)^2$$

for the case of a weak object with a Gaussian type feature. In the case when the detector resolution is much poorer than the source resolution which is the case for point projection type imaging as opposed to synchrotron imaging, ie $\sigma_d \gg \sigma_s$, the optimum magnification is large, $M \gg 1$. For the case found in this thesis that the optimum magnification was around 13, and source size around 4 $\mu$m, the detector resolution would need to be about 14 $\mu$m. Although the high resolution image plate (FDL-URV) is capable of 25 $\mu$m resolution with the Fuji BAS-5000, subsequent scattering of the stimulating light within components of the active layer (see Seggern [160]), expands this to between 100-170 $\mu$m depending on the system (see Amemiya [188], [189]). For the system used here, a resolution around 150-160 would bring the theoretical values to a factor of 2 greater than experiment.

For implementation into clinical practice, besides the resolution requirements, the flux of a micro-focus type source is insufficient for reasonable time constraints. The phase contrast requirements are unfortunately competing against SNR requirements and patient dose. A good discussion of these parameters can be found in Gureyev [186], along with various alternative sources such as rotating anode sources, laser plasma sources and inverse Compton sources, which may overcome the flux limitation. Of particular interest are the liquid jet x-ray sources at KTH in Stockholm, by Otendal et al [190], with a factor of 10-1000 times higher brilliance than current compact sources. Combined with a photon counting type detector such as PILATUS, Henrich et al [191], would open up the potential of phase contrast imaging to be a feasible technique along side conventional absorption based radiography for better diagnostic imaging.
Bibliography


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