1 Introduction

1.1 Direct Problem: Phase Contrast Image Formation

1.1.1 Basic X-ray Illumination Physical Model

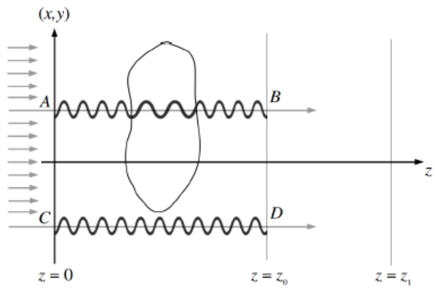


Figure 1.1: Basic X-ray Illumination Model [1]

For phase retrieval, I will start with the direct problem. Consider Fig.1.1. Here, z-directed monochromatic complex scalar X-ray waves illuminate a static non-magnetic object, from the left. By assumption, the object is totally contained within the slab of space between $z = 0$ and $z = z_0 \geq 0$ [1].We assume the original incident wave on the left hand side of $z = 0$ has a uniform flux. Due to the weak interaction of X-rays with matter, the propagation path inside the object can be assumed to be straight, that is to say that diffraction within the object is neglected [4]. This is the so-called projection approximation. When the wave reaches the position $z = z_0$, which is the exit plane of object, meaning it has transmitted through the object, the wave propagation can be modeled as diffraction between exit plane position $z = z_0$ and detector position $z = z_1$. For the near-field diffraction, we can make use of Fresnel diffraction which is based on Fresnel approximation. For the far-field diffraction, we can make use of Fraunhofer diffraction which is based on Fraunhofer approximation.

1.1.2 Complex Refractive Index and Transmittance Function

Consider Fig.2, we wish to determine the complex disturbance (wave function) over the plane $z = z_0$, which is termed the exit plane of the object, as a function of both (i) the complex disturbance over the entrance plane $z = 0$ and (ii) the refractive index distribution of the object[1].

By citing the formula from [1], under the projection approximation,

$$\tilde{u}(x, y, z = z_0) \approx \exp\{\frac{k}{2\pi}\int_{z=0}^{z=z_0}[1 - n^2(x, y, z)]dz\}\tilde{u}(x, y, z = 0) \tag{1.1}$$

Basically the direct problem describes the image formation. The optical properties of the object can be described by its 3D complex refractive index distribution:

$$n(x, y, z) = 1 - \delta_r(x, y, z) + i\beta(x, y, z) \tag{1.2}$$

where δ_n is the refractive index decrement distribution, β the absorption index, (x, y, z) are the spatial coordinates. The real part corresponds to the refractive index. We shall see that the imaginary part of this complex refractive index can be related to the absorptive properties of a sample. And we have

$$|\delta_n(x, y, z)|, |\beta(x, y, z)| \ll 1 \tag{1.3}$$

since the complex refractive index for hard X-rays is typically extremely close to unity. Hence:

$$1 - n(x, y, z)^2 \approx 2[\delta_n(x, y, z) - i\beta(x, y, z)] \tag{1.4}$$

where we have discarded terms containing δ_n^2, β_n^2 and $\delta_n^2\beta_n^2$ since these will be much smaller than the terms that have been retained in the right side of Eq.1.4.

If the above expression is substituted into Eq.1.1, we obtain

$$\tilde{u}(x,y,z=z_0) \approx \tilde{u}(x,y,z=0) \times \exp\{-i\frac{2\pi}{\lambda}\int_{z=0}^{z=z_0}[\delta_n(x,y,z) - i\beta(x,y,z)]dz\}, \lambda = \frac{2\pi}{k} \tag{1.5}$$

This shows that the exit wave field $\tilde{u}(x,y,z=z_0)$ may be obtained from the entrance wave field $\tilde{u}(x,y,z=0)$ via multiplication by a transmission function $T(x,y)$. The transmission function is the second term of Eq.1.5.

Hence, the position-dependent phase shift due to the object is:

$$\varphi(\mathbf{x}) = (-2\pi/\lambda)\int \delta_n(x,y,z)dz \tag{1.6}$$

Here, $\mathbf{x} = (x,y)$ are the spatial coordinates in the plane perpendicular to the propagation direction z.

The above expression quantifies the deformation of the X-ray wave-fronts due to passage through the object. Physically, for each fixed transverse coordinate (x,y), phase shifts (and the associated wave-front deformations) are continuously accumulated along energy-flow streamlines (loosely, "rays") such as AB in Fig.1.2.

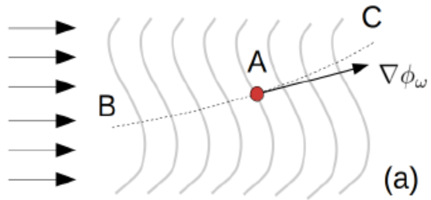


Figure 1.2: X-ray wave-fronts

At a given instant of time $t = t_0$, the intensity of an X-ray field is $I(x,y,z,t=t_0)$. The wave-fronts, namely the surfaces of constant phase at time = t_0, are indicated by the series of curved surfaces. At any point A the wave-fronts move away from the source as time increases. The direction of energy flow at point A is $\bigtriangledown\phi(x,y,z,t=t_0)$ [1]

The attenuation may be obtained by taking the squared modulus of Eq.1.5, to give the Beer Lambert law.

The squared modulus of $\tilde{u}(x,y,z)$ gives the intensity value,i.e.$I(x,y,z=z_0)$

$$\begin{aligned} I(x,y,z=z_0) = I(x,y,z=0) \times \left|\exp[-2k\int_{z=0}^{z=z_0}\beta(x,y,z)dz]\right| \times \left|\exp[-i2k\int_{z=0}^{z=z_0}\delta_n(x,y,z)dz]\right| \\ = I(x,y,z=0) \times \left|\exp[-2k\int_{z=0}^{z=z_0}\beta(x,y,z)dz]\right| \end{aligned} \tag{1.7}$$

From Eq.1.7, we can see the real part of complex refractive index δ_n, i.e. the refractive index decrement will not be reflected by the value of the intensity because it is present in imaginary power factor of the third term that is equal to 1. While the imaginary part of the complex refractive index β_n, i.e. the absorption index, can be reflected by the intensity. That's why in classical computed tomography, we make use of attenuation as the parameter to be inverted (inverse radon transform) directly.

So, if we take the log operator on both sides of equation Eq.1.7,we have:

$$\log_e \frac{I(x,y,z=z_0)}{I(x,y,z=0)} = -\int_{z=0}^{z=z_0} 2k\beta(x,y,z)dz = -\int_{z=0}^{z=z_0} udz \tag{1.8}$$

where $u = 2k\beta(x,y,z)$ is the linear attenuation coefficient

So, for the attenuation, we can obtain

$$B(\mathbf{x}) = (2\pi/\lambda)\int \beta(x,y,z)dz \tag{1.9}$$

Here, $\mathbf{x} = (x,y)$ are the spatial coordinates in the plane perpendicular to the propagation direction z.

Both the attenuation and the phase shift induced by the object can be described as projections through the absorption and refractive index distributions respectively.

We assume that the object can be described as a 2D complex transmittance function $T(\mathbf{x})$, that is the propagation path inside the object is considered straight and propagation effects that occur inside the sample are neglected. In reality, wave propagation inside the object is not ideally straight, but the deflection angle is too tiny that can be ignored. This transmittance function can be written as:

$$T(\mathbf{x}) = exp[-B(\mathbf{x})]exp[i\varphi(\mathbf{x})] \tag{1.10}$$

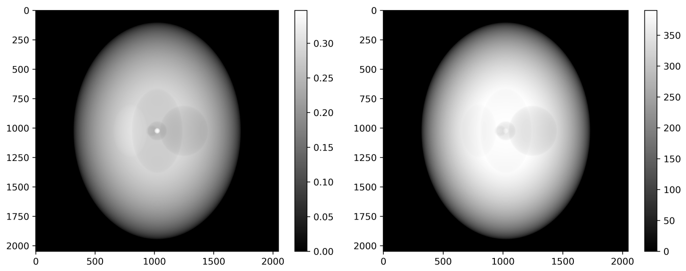
Finally, we have

$$u_0(\mathbf{x}) = T(\mathbf{x}) \times u_{inc}(\mathbf{x}) \tag{1.11}$$

Here, $u_0(\mathbf{x})$ is the wave field at the exit plane of the object while $u_{inc}(\mathbf{x})$ is the original incident wave to object.

The Fresnel diffraction after the sample and propagation-based phase contrast are detailed in the Appendix.

1.1.3 Necessity of Phase Retrieval



(a) Attenuation Projection (b) Phase Projection

Figure 1.3: Projection Image

The main interest in this technique is the several orders of magnitude increase in sensitivity compared with standard, attenuation-based tomography

Apparently the gray level range of phase projection is thousands times larger than that of attenuation projection, it means the phase projection has more contrast than attenuation projection practically. That's the interest brought by phase projection in computed tomography. The phase shift can be obtained with phase retrieval from the measured intensity I after the Fresnel diffraction of the wave.

1.1.4 Linear Fresnel Transform and Its Representation in Spatial and Fourier Domain

With Eq.6.6 (see appendix), Rayleigh-Sommerfield diffraction integral is a linear integral transform, we can treat the wave propagation from one point to another point as a linear transformation. Therefore, in terms of the exit wave, free space propagation can be considered a linear operator, and when moving the detector a relatively short distance downstream from the sample, the intensity is called a Fresnel diffraction pattern. So, the effect on the wave of letting it propagate in free space by Fresnel propagator can be described as a convolution [4]:

$$u_D(\mathbf{x}) = P_D(\mathbf{x}) * u_0(\mathbf{x}) \tag{1.12}$$

is the complex wave function in the diffraction plane, a distance D from the object and $P_D(\mathbf{x})$ is called the Fresnel propagator. And the Fresnel integral above can be seen as a convolution of the exit wave $u_0(\mathbf{x})$ and a propagator. The Fresnel propagator in the spatial domain can be written[4]:

$$P_D(\mathbf{x}) = \frac{1}{i\lambda D} \exp\left(i \frac{\pi}{\lambda D} |\mathbf{x}|^2\right) \tag{1.13}$$

where we have dropped the non-relevant phase factor. By Fourier transform, Fresnel propagator expression in Fourier domain is [4]:

$$\tilde{P_D}(\mathbf{f}) = \exp\left(-i\pi\lambda D \, |\mathbf{f}|^2\right) \tag{1.14}$$

The representation of wave propagation in Fourier domain is: [4]

$$\tilde{u}_D(\mathbf{f}) = \tilde{P}_D(\mathbf{f}) \times \tilde{u}_0(\mathbf{f}) \tag{1.15}$$

1.1.5 Phase Contrast Image for incident wave to object as uniform flux

The phase contrast is generated simply by letting the beam propagate in free space a relatively short distance after interaction with the object. The measured intensity can be modelled in the Fresnel diffraction formalism; hence, the images recorded can be called Fresnel diffraction patterns.

The recorded intensity on the detector is the squared modulus of the exit wave,

$$I_D(\mathbf{x}) = |T(\mathbf{x}) * P_D(\mathbf{x})|^2 \tag{1.16}$$

where $T(\mathbf{x})$ is the transmittance function and P_D is the Fresnel propagator as above with distance D as parameter. As mentioned in previous part, $u_0(\mathbf{x}) = T(\mathbf{x})\ u_{inc}(\mathbf{x})$. Because we assume the original incident wave $u_{inc}(\mathbf{x})$ has uniform flux, the wave field at the exit plane of object $u_0(\mathbf{x})$ would be $T(\mathbf{x})$, this is the basic and critical assumption made in our model. And the propagation of a wave in free space can also be calculated in the Fourier domain. It is given by [4]:

$$I_D(\mathbf{x}) = \left| \mathscr{F}^{-1}[\int T(\mathbf{x} - \frac{\lambda D\mathbf{f}}{2}) T^*(\mathbf{x} + \frac{\lambda D\mathbf{f}}{2}) \exp(-i2\pi \mathbf{x} \cdot \mathbf{f})] \right|^2 \tag{1.17}$$

Alternatively,the Fourier transform of intensity of Fresnel diffraction pattern can be written as: [4]

$$\tilde{I}_D(\mathbf{f}) = \int T(\mathbf{x} - \frac{\lambda D\mathbf{f}}{2}) T^*(\mathbf{x} + \frac{\lambda D\mathbf{f}}{2}) \exp(-i2\pi \mathbf{x} \cdot \mathbf{f}) d\mathbf{x} \tag{1.18}$$

which will be used as the starting point for the inverse problem in the following.

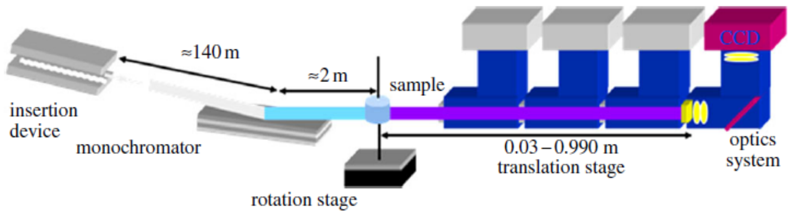
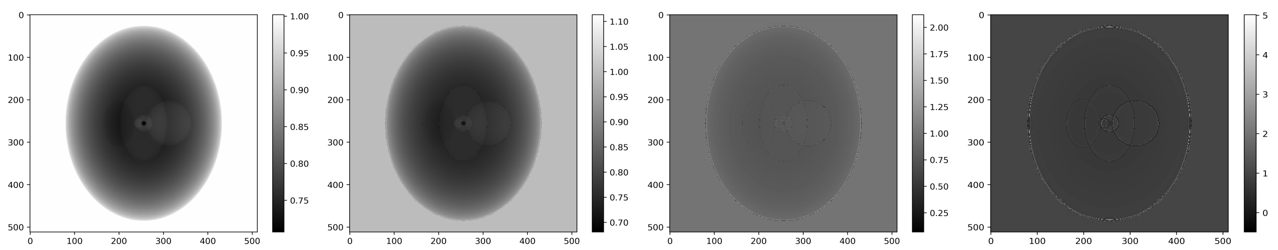


Figure 1.4: Experimental set-up [2]

1.1.5.1 Phase Contrast Image of different distances

oversampling rate	energy of photon(keV)	pixel size(m)
4	24	$7.5/4 \times 10^{-6}$

Table 1.1: Parameter of Phase Contrast Image Formation



(a) Phase Contrast Image of distance 0.0m (b) Phase Contrast Image of distance 0.01m (c) Phase Contrast Image of distance 0.1m (d) Phase Contrast Image of distance 1.0m

Figure 1.5: Phase Contrast Image of different distances

As shown in (a), if the object-to-detector propagation distance is zero, however, one has a contact image that displays no propagation-based X-ray phase contrast [1] . Phase and amplitude information at the object exit plane will be entangled in intensity measurements downstream of the object. From (b) to (d), there is more and more phase contrast in phase contrast images as the distance increases, and apparently the gray level range is gradually increased. Using these diffraction patterns directly as input to a tomographic reconstruction algorithm yields an edge enhancement effect owing to the phase contrast and is called phase-contrast tomography

1.2 Inverse Problem - Phase Retrieval

1.2.1 Contrast Transfer Function Based on Linearization of Transmittance Function

Estimating the phase shift from these diffraction patterns intensity is called phase retrieval. The retrieved phase shift can be used in conjunction with tomography to reconstruct the 3D refractive index. This process is called 3D phase contrast tomography or holotomography.[4]

In this estimation problem, we will estimate the unknown absorption $\tilde{B}$ and phase shift $\tilde{\varphi}$ only based on $\tilde{I}(\mathbf{f})$ that represents the practical measured(detected) Fresnel diffraction intensity map. By Eq.18, since $\tilde{I}(\mathbf{f})$ can be deduced from the transmittance function T with known fixed parameter λ and variable distance D, and since by Eq.17, the transmittance function T could be expressed as a function of $\tilde{B}(\mathbf{f})$ and of the phase shift $\tilde{\varphi}(\mathbf{f})$, it means we can solve the inverse problem by least square minimization. In the Fourier domain, we are trying to minimize the distance between Fresnel diffraction intensity map $\left|\mathbf{Fr}_D[\tilde{T}(\mathbf{f})]\right|^2$ and Fourier transform form of practical measured(detected) Fresnel diffraction intensity map $\tilde{\mathbf{I}}(\mathbf{x})$,i.e.$\tilde{\mathbf{I}}(\mathbf{f})$ so that we could optimize the solutions for the unknown absorption $\tilde{B}(\mathbf{f})$ and phase shift $\tilde{\varphi}(\mathbf{f})$.

The phase retrieval from one or several Fresnel diffraction patterns can be defined as the least square minimization problem in the image space:[4]

$$\varphi(\mathbf{x}) = \arg\min_{\varphi} \sum_D \left| \quad |\mathbf{Fr}_D[T(\mathbf{x})] \quad |^2 - \mathbf{I}_D(\mathbf{x}) \right|^2, D \in \{D_1, D_2, D_3, ..., D_N\} \tag{1.19}$$

where $\mathbf{Fr}_D$ is the operator symbol of the Fresnel transform with parameter D.

However, we will solve this kind of least square minimization problem in Fourier domain: [4]

$$\tilde{\varphi}(\mathbf{f}) = \arg\min_{\varphi} \sum_D \left| \quad \left|\mathbf{Fr}_D[\tilde{T}(\mathbf{f})] \quad \right|^2 - \tilde{\mathbf{I}}_D(\mathbf{f}) \right|^2, D \in \{D_1, D_2, D_3, ..., D_N\} \tag{1.20}$$

The reason for including several distances in Eq.19 is that the transfer function to a certain distance for the Fresnel transform can have zero crossings. This means that information at these frequencies in the Fourier transform of the phase functions will not contribute to the diffraction pattern at that distance. This means that several distances have to be combined to give as good coverage of the Fourier domain as possible. [4]

The contrast transfer function method is based on an assumption of weak absorption and slowly varying phase shift. Since both the absorption $\tilde{B}$ and phase shift $\tilde{\varphi}$ are the power factors of in the expression of transmittance function $T(\mathbf{x})$, to make them be involved in Eq.19 directly, we can take them out from the power factor by linearizing the transmittance $T(\mathbf{x})$. The forward model is linearized by Taylor expanding the transmittance function Eq.17 to the first order, [4]

$$T(\mathbf{x}) \approx 1 - B(\mathbf{x}) + i\varphi(\mathbf{x}) \tag{1.21}$$

Substituting into Eq.18 and again keeping only first order terms gives

$$\tilde{I}_D(\mathbf{f}) = \delta(\mathbf{f}) - 2\cos(\pi\lambda D\,|f|^2)\tilde{B}(\mathbf{f}) + 2\sin(\pi\lambda D\,|f|^2)\tilde{\varphi}(\mathbf{f}) \tag{1.22}$$

where $\delta(f)$ is the unit impulse function, $\tilde{B}(f)$ is the Fourier transform of the absorption and $\tilde{\varphi}(f)$ is the Fourier transform of the phase. Although this expression is obtained by assuming weak object interaction, it can be shown to be valid for weak absorption and slowly varying phase.[4]

$$B(\mathbf{x}) \ll 1, \quad |\varphi(\mathbf{x}) - \varphi(\mathbf{x} + \lambda D\mathbf{f})| \ll 1 \tag{1.23}$$

Since the phase contrast factor before $\tilde{\varphi}(\mathbf{f})$ in Eq.20 has zero crossings, several distances have to be used in order to cover as much of the Fourier domain as possible. Then, Eq.22 is used to set a linear least squares optimization problem, taking the different distances into account: [4]

$$min\epsilon = \sum_D \left| 2\sin(\pi\lambda D\,|\mathbf{f}|^2)\tilde{\varphi}(\mathbf{f}) - 2\cos(\pi\lambda D\,|\mathbf{f}|^2)\tilde{B}(\mathbf{f}) - \tilde{\mathbf{I}}_D(\mathbf{f}) \right|^2 \tag{1.24}$$

The solution for the phase if $\mathbf{f} \neq (0,0)$ is: [4]

$$\tilde{\varphi}(f) = \frac{1}{2\Delta + \alpha}[C\sum_D \tilde{\mathbf{I}}_D(\mathbf{f})\sin(\pi\lambda D\mathbf{f}^2) - A\sum_D \tilde{\mathbf{I}}_D(\mathbf{f})\cos(\pi\lambda D\mathbf{f}^2)] \tag{1.25}$$

with $A = \sum_D \sin(\pi\lambda D\mathbf{f}^2)\cos(\pi\lambda D\mathbf{f}^2)$, $B = \sum_D \sin^2(\pi\lambda D\mathbf{f}^2)$, $C = \sum_D \cos^2(\pi\lambda D\mathbf{f}^2)$ and $\Delta = BC - A^2$. α is a regularization parameter, introduced by Tikhonov regularization (Tikhonov and Arsenin, 1977) of Eq.22. This is chosen to minimize the standard deviation outside the imaged object at one projection angle, and then used for the whole tomographic data set[1]. From Eq.25 it can be seen that solving for the phase requires $N + 1$ calculations of 2D FFTs, one forward of each image at each distance (N) and one inverse to get the phase. Typically, three or four distances are used.