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Limitations imposed by specimen phase gradients on the design of grating based x-ray phase contrast imaging systems

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Abstract

X-ray phase contrast imaging is a very promising technique that may lead to significant advancements in a variety of fields, perhaps most notably, medical imaging. The radiation physics group at University College London is currently developing an x-ray phase contrast imaging technique that works with laboratory x-ray sources. This system essentially measures the degree to which photons are refracted by regions of an imaged object. The amount of refraction that may be expected to be encountered in practice impacts strongly upon the design of the imaging system. In this paper, we derive an approximate expression between the properties of archetypal imaged objects encountered in practice and the resulting distribution of refracted photons. This is used to derive constraints governing the design of the system.

1. Introduction

It is hoped that x-ray phase contrast imaging (XPCi) will revolutionize a variety of x-ray imaging applications, such as medical, security, and industrial inspection. Techniques such as Talbot interferometry [1] and Talbot–Lau interferometry [2] have been used to obtain stunning phase contrast images employing laboratory sources of high spatial coherence or effective sources of high spatial coherence achieved through the use of a source grating. Our group is currently developing a technique that employs coded apertures to perform XPCi using sources of lower spatial coherence than Talbot and Talbot–Lau interferometry [3]. The coded aperture imaging system is depicted schematically in Fig. 1. Such a system permits the acquisition of images under bright-field, dark-field, and intermediate illumination conditions as determined by the offset of the detector apertures relative to the projection of the sample apertures, denoted ΔP in Fig. 1. Such a system could be implemented using a single sample/detector aperture in which the imaged object is scanned in order to obtain an image of the entire object. However, in order to reduce the need for object scanning, a number of such apertures is employed in parallel such that several regions of the object may be imaged simultaneously. Such an approach may, however, lead to spurious details in acquired profiles, as illustrated in Fig. 2. The profile contains a spurious peak that results from photons being refracted from one of the parallel pairs of sample and detector apertures into another. Such a spurious peak could create an ambiguity in an XPCi image and mask weak phase gradients.

In this paper we derive constraints on the periodicity (P) of the sample/detector apertures and ΔP , under which the multi-aperture imaging system may be considered approximately

equivalent to the single aperture imaging system. The analysis is performed for coded aperture XPCi systems; however, the results are relevant to the aforementioned alternative techniques. This paper begins by developing an approximate expression for the intensity of x-rays refracted by a cylindrical object. This result is then used to calculate constraints on P and ΔP . A cylindrical object is employed because any smooth curve may be approximated locally by a circle of appropriate radius.

2. Approximation of the Field Incident upon the Detector

We start with the coded aperture XPCi system depicted in Fig. 1. Fresnel–Kirchhoff diffraction theory [4] can be used to write the field incident upon the detector apertures at position Q due to a monochromatic point source located at $\bar{x} = x_s$ as $U(Q) = U_{in}(Q) + U_s(Q)$, where U_s is the scattered field defined by

$$U_s(Q) = C \int_{\mathcal{O} \cap \mathcal{A}} [\exp(i\phi(\xi)) - 1] \times \exp\left(ik\xi^2 \frac{M}{2z_{od}} - ik\xi \frac{x'}{z_{od}}\right) d\xi, \quad (1)$$

where C is a complex constant, $\mathcal{O}$ is the extent of the object, $\mathcal{A}$ is the transmitting part of the sample apertures, $\phi(\xi) = k \int_{\mathcal{O}} n(\xi, z) dz$ is the optical thickness of the object, $k = 2\pi/\lambda$, λ is the wavelength of the source, n is the refractive index of the object, U_{in} is the field incident directly on the detector apertures in the absence of an object, $x' = x + x_s z_{od}/z_{so}$, $M = (z_{so} + z_{od})/z_{so}$ is the magnification, i is the imaginary unit, and the remaining terms are defined in Fig. 1. This expression is explained in more detail in a recent publication [5]. The model is extended to consider a polychromatic source of finite width later in this section.

The performance of the system is strongly influenced by the displacement, ΔP , between the detector apertures and the projection of the sample apertures. Contrast increases, at the expense of signal, as the degree of overlap between transmitting regions of the sample and detector apertures decreases. One may consider the sample and detector apertures to be composed of a combination of individual apertures defined mathematically as

$\mathcal{A} = \sum_j \mathcal{A}_j(\xi - \Delta A)$ and $\mathcal{D} = \sum_j \mathcal{D}_j(x - M\Delta A - \Delta P)$ respectively, where

$$\begin{aligned} \mathcal{A}_i(\xi) &= \begin{cases} 1 & \frac{jP}{M} - \frac{\eta P}{2M} < \xi < \frac{jP}{M} + \frac{\eta P}{2M} \\ 0 & \text{otherwise} \end{cases}, \\ \mathcal{D}_j(x) &= \begin{cases} 1 & jP - \frac{\eta P}{2} < x < jP + \frac{\eta P}{2} \\ 0 & \text{otherwise} \end{cases}, \end{aligned} \quad (2)$$

η is the fill factor of the apertures, and ΔA is a shift imparted on the entire imaging system.

We seek to determine the conditions under which an object, or part of an object, illuminated within aperture $\mathcal{A}_j$ causes a significant signal to be detected in an aperture adjacent to $\mathcal{D}_j$. The curvature of any smooth surface may be described locally by a circle and so we employ a cylinder, with its axis perpendicular to both the ξ and z axes, as our imaged object. We consider a nonabsorbing cylinder as x-ray refraction is due to gradients in the real part of the refractive index, which we denote $n = 1 - \delta$, where δ is the refractive index decrement, typically of the order of 10^{-6} to 10^{-7} for materials at x-ray photon energies. The phase

function of the cylinder is thus given by $\phi(\xi) = -2k\delta \sqrt{R^2 - \xi^2}$, where R is the cylinder radius and it has been assumed that the cylinder is positioned with its center at $\xi = 0$. This places no restriction upon the final result as it is assumed that the edge of the cylinder lies within a transmitting region of the sample apertures, $\mathcal{A}_j$, for some j .

Returning to the ultimate goal of the paper, we seek to determine the minimum separation between the geometrical projection of $\mathcal{A}_j$ and an adjacent detector aperture $\mathcal{D}_{j+1}$ such that very little signal is detected in $\mathcal{D}_{j+1}$ due to x-rays originating in $\mathcal{A}_j$. We consider a worst-case scenario in which the sample apertures are positioned such that the upper limit of one of the transmitting regions is equal to R , i.e.,

$$\frac{jP}{M} + \frac{\eta P}{2M} - \Delta A = R, \quad (3)$$

for some choice of j and ΔA . We opt to shift the imaging system rather than the object as this simplifies the following analysis. To further simplify the problem, we consider the sample apertures to consist of only the aperture $\mathcal{A}_j$, satisfying Eq. (3).

We are interested in evaluating $|U_{\text{in}} + U_s|^2 - |U_{\text{in}}|^2$ for x in the geometrical shadow of $\mathcal{A}_j$,

i.e., $x > jP + \frac{\eta P}{2} - M\Delta A$. U_{in} is nonzero in this region only due to diffraction and contributes only to the flat-field image. Furthermore, it rapidly decays in this region. It is thus reasonable, as will be verified later, to consider $|U_s|^2$ as the primary contribution of the object induced perturbation to x-ray intensity in this region. U_s , in Eq. (1), could be evaluated numerically; however, it is much more instructive to determine an approximate solution for large angles of refraction for general values of δ and R . We have shown, in a recent paper [5], that the refracted field in the geometrical shadow of the cylinder may be approximated to the first order by using the stationary phase approximation as

$$U_s(x') \sim C \sqrt{\frac{2\pi}{k|\ddot{g}_1(x', \xi_0)|}} \exp\left(i\left[kg_1(x', \xi_0) + \frac{\pi}{4}\right]\right), \quad (4)$$

where

$$g_1(x', \xi) = \frac{M\xi^2}{2z_{od}} - \frac{x'\xi}{z_{od}} - 2\delta\sqrt{R^2 - \xi^2},$$

ξ_0 is obtained as the unique solution of $\dot{g}_1(x', \xi_0) = 0$, and all derivatives of g_1 are with respect of ξ . By substituting $\xi_\epsilon = R(1 - \epsilon)$, for small $\epsilon > 0$, an approximate solution for $\dot{g}_1(x', R(1 - \epsilon)) = 0$ is obtained as $x' \approx MR + 2\delta z_{od} / \sqrt{2\epsilon}$ or $\epsilon \approx 2z_{od}^2 \delta^2 / (x' - MR)^2$. Substituting this value of ξ_ϵ into Eq. (4) allows us to approximate $|U_s(x')|^2$ as

$$|U_s(x')|^2 \approx |C|^2 \frac{\lambda}{\frac{M}{z_{od}} + \frac{2\delta}{R} \left[\frac{(x' - MR)^3}{(2z_{od}\delta)^3} + \frac{x' - MR}{2z_{od}\delta} \right]}. \quad (5)$$

It is easy to show that, if the entire cylinder were illuminated, the peak of $|U_s|^2$ is given by $|U_1^p|^2 = |C|^2 \lambda z_{od} R / (MR + 2\delta z_{od})$ and so we can write the intensity of the refracted field, normalized by its peak, as

$$I_N(x') = \frac{MR + 2\delta z_{od}}{MR + 2\delta z_{od} \left[\left(\frac{x' - MR}{2z_{od}\delta} \right)^3 + \frac{x' - MR}{2z_{od}\delta} \right]}. \quad (6)$$

which is valid only for $x' \gg MR$. We are interested, then, in when the refracted field reaches a fraction, ξ , of its peak and so we write $x' = RM + \Delta x + x_s z_{od}/z_{so}$, which, upon substitution into $I_N(x') = \xi$, yields

$$y^3 + y = \frac{1}{\xi} + \frac{MR(1/\xi - 1)}{2\delta z_{od}}, \quad (7)$$

where $y = (\Delta x + x_s z_{od}/z_{so})/(2z_{od}\delta)$. This polynomial may be solved for the value Δx , which establishes a limit on how close $\mathcal{D}_{j+1}$ may be positioned to the geometrical projection of $\mathcal{A}_j$ in order to not detect a significant signal from x-rays originating in $\mathcal{A}_j$. A source of full width at half-maximum W may be modeled by assuming the worst case of $x_s = -W/2$. It is also noted that this result is independent of the wavelength and so is valid for polychromatic sources. Finally, we note that we have quoted, without derivation, a result similar to that of Eq. (7) in a recent paper [5]. This previous result was, however, found to be an oversimplification of the problem as the term linear in y was omitted. We publish this paper to present the correct result and its derivation.

3. Results

Figure 3 contains a collection of plots comparing $|U_{in}(x') + U_s(x')|^2 - |U_{in}(x')|^2$ (normalized by the same factor as $I_N(x')$) with $I_N(x')$ for a variety of radii and δ values expected to be encountered in practice. The plots show that the approximation is reasonable, particularly for larger values of δ , which we are most interested in. The approximation remains valid for intermediate radii and δ values not shown in Fig. 3.

Having demonstrated the validity of the approximation used to derive the result of Eq. (7), we can now calculate Δx for a range of radii and δ values. Figure 4 shows contours of Δx for such a range of values expected to be encountered in practice and $\xi = 0.01$. The figure demonstrates that Δx increases when either δ or the radius of curvature increases. The contours show that a degree of crosstalk between $\mathcal{A}_j$ and $\mathcal{D}_{j+1}$ will be inevitable for typical coded aperture XPCi systems, as a small detector pixel dimension is sought to increase the resolution of the acquired image without the need to scan the imaged object. Flat panel detectors are available with a pixel dimension P as small as $50 \mu\text{m}$ (Hamamatsu C9732DK passive pixel CMOS flat panel). With Δx approaching the detector periodicity it is necessary to either skip alternate pixels or use a low fill factor in order to minimize crosstalk between nonmatching sample/detector aperture pairs. The ramifications of this result may, however, be more problematic for the related Talbot and Talbot–Lau type XPCi imaging systems (see Refs. [2,6], for example) as these employ detector gratings with a substantially smaller periodicity.

The results derived in this paper thus allow the derivation of a design rule for aperture periodicity for coded aperture, Talbot, and Talbot–Lau type XPCi imaging systems. For coded aperture systems, it also provides a constraint on the separation between sample and detector apertures.

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Fig. 1.

System diagram of an XPCi system employing a point source. P is the detector pixel width and ΔP is the displacement of the detector aperture/detector arrangement relative to the rojection of the sample apertures. The detector apertures are always centered upon the detector pixels. The object to be imaged would normally be placed adjacent to the sample apertures on the detector side.

Fig. 2.

Sample profile of a cylinder with radius 0.5 mm, $\delta = 10^{-6}$, $P = 100 \mu\text{m}$, $\Delta P = P/4$, x-ray photon energy 17.5 keV, $z_{\text{so}} = 1.6 \text{ m}$, $z_{\text{od}} = 0.4 \text{ m}$, and a scanning step size of $2 \mu\text{m}$. The plot shows a spurious positive peak, indicated by a box, resulting from refracted x-rays, which are detected by a pixel not matched with the part of the sample aperture through which the x-rays entered the system.

Fig. 3.

(Color online) Plots of $|U_{\text{in}}(x') + U_s(x')|^2 - |U_{\text{in}}(x')|^2$ (solid curve, normalized by $|U_1^P|^2$) and $I_N(x')$ (broken curve) for a variety of values of δ and R . The left- and right-hand columns correspond to delta values of 10^{-6} and 10^{-7} , respectively. The rows correspond to values of radii, from the top down, of 10, 100, and 1000 μm , respectively. Note that $|U_{\text{in}}(x') + U_s(x')|^2 - |U_{\text{in}}(x')|^2$ is highly oscillatory and is plotted with equal line widths in each set of axes. These results were obtained for a detector periodicity, P , of 85 μm , $\eta = 0.5$, $z_{\text{so}} = 1.6$ m, and $z_{\text{od}} = 0.4$ m. These values match our experimental setup, but the correspondence shown above does not depend on these values.

Fig. 4. Contours of Δx for a range of radii and values of δ for a threshold of $\xi = 0.01$.