A general theory of interference fringes in x-ray phase grating imaging

Aimin Yan and Xizeng Wu^{a)}

Department of Radiology, University of Alabama at Birmingham, Birmingham, Alabama 35249

Hong Liu^{a)}

Center for Bioengineering and School of Electrical and Computer Engineering, University of Oklahoma, Norman, Oklahoma 73019

(Received 17 October 2014; revised 1 May 2015; accepted for publication 4 May 2015; published 26 May 2015)

Purpose: The authors note that the concept of the Talbot self-image distance in x-ray phase grating interferometry is indeed not well defined for polychromatic x-rays, because both the grating phase shift and the fractional Talbot distances are all x-ray wavelength-dependent. For x-ray interferometry optimization, there is a need for a quantitative theory that is able to predict if a good intensity modulation is attainable at a given grating-to-detector distance. In this work, the authors set out to meet this need.

Methods: In order to apply Fourier analysis directly to the intensity fringe patterns of two-dimensional and one-dimensional phase grating interferometers, the authors start their derivation from a general phase space theory of x-ray phase-contrast imaging. Unlike previous Fourier analyses, the authors evolved the Wigner distribution to obtain closed-form expressions of the Fourier coefficients of the intensity fringes for any grating-to-detector distance, even if it is not a fractional Talbot distance.

Results: The developed theory determines the visibility of any diffraction order as a function of the grating-to-detector distance, the phase shift of the grating, and the x-ray spectrum. The authors demonstrate that the visibilities of diffraction orders can serve as the indicators of the underlying interference intensity modulation. Applying the theory to the conventional and inverse geometry configurations of single-grating interferometers, the authors demonstrated that the proposed theory provides a quantitative tool for the grating interferometer optimization with or without the Talbot-distance constraints.

Conclusions: In this work, the authors developed a novel theory of the interference intensity fringes in phase grating x-ray interferometry. This theory provides a quantitative tool in design optimization of phase grating x-ray interferometers. © 2015 American Association of Physicists in Medicine. [<http://dx.doi.org/10.1118/1.4921124>]

Key words: x-ray imaging, phase contrast imaging, phase grating, x-ray interferometry

1. INTRODUCTION

In recent years, phase-contrast x-ray imaging has become an active research field. In contrast to conventional x-ray imaging such as radiography and computed tomography, phase-contrast imaging relies on the x-ray phase shifts that tissue can generate. The amount of x-ray phase shift Φ is determined by the integral of tissue electron density over the ray path as $\Phi = -\lambda r_e \int \rho_e ds$, where λ is the x-ray wavelength, r_e the classical electron radius, and ρ_e denotes tissue electron density. In the x-ray energy range of 5–200 keV, the differences in x-ray phase shifts between tissues are about one thousand times greater than their differences in the projected linear attenuation coefficients.^{1,2} Therefore, phase-contrast imaging has the potential to greatly increase x-ray detection sensitivity. X-ray grating interferometry, such as Talbot interferometry, is a differential phase-contrast imaging technique that has received a lot of attention in recent years.^{3–16} Figure 1 shows a schematic of such a phase grating x-ray interferometer with a microfocus source. To outline its imaging principle, we first consider the case without a sample. The grating is a periodic

array of phase shift modulation, and it serves as a beam splitter that divides the incident beam into different diffraction orders. The interference between diffraction orders generates intensity fringes with their shape and modulation dependent on the grating-to-detector distance. The grating self-images with the maximal intensity modulation are formed only at some discrete distances, which are called the fractional Talbot distance.^{5–7} As is well known, for one-dimensional (1-D) phase gratings, the fractional Talbot distances associated with monochromatic parallel x-ray beams are given as

$$Z_{F-1D} = (2k - 1)p_1^2 / (2\lambda\eta^2), \quad (1)$$

where p_1 is the period of the phase grating, $\eta = 2$ for 1-D π -shift gratings, $\eta = 1$ for 1-D $\pi/2$ -shift gratings, and k defines the order of the fractional Talbot distance and $k = 1, 2, 3, \dots$ ^{5–7} With the presence of a sample, the Talbot self-image fringes will be distorted and encoded with the sample's attenuation and phase shifts. For example, the phases of the fringe's frequency components are to be encoded with the differentials of the sample's phase map Φ . Subsequent phase retrieval is required to extract the sample's phase map from

FIG. 1. Schematic of an x-ray phase grating interferometer with a microfocus source.

the intensity fringes. The phase retrieval is implemented by using two methods: the phase stepping method and the Fourier spectrum analysis method, as is discussed in details in the literature.^{7-9,17-19}

In medical imaging applications, broadband polychromatic x-ray sources such as x-ray tubes are employed. With polychromatic x-ray, the concept of Talbot distances itself is not well defined for two reasons. First, the Talbot distances are wavelength-dependent. A given grating–detector distance may fall into a Talbot distance with one wavelength but just mismatch the Talbot distance with the others. Second, the Talbot distances depend on the phase shift value of a grating as well; however, the phase shift value of the grating varies with x-ray wavelengths. For example, a π -grating for 20-keV x-ray becomes a $\pi/2$ -grating for 40-keV x-ray. Consequently, using a broad band x-ray beam would stretch the self-image regime into several distance intervals rather than exhibiting sharp discrete fractional Talbot distances. On the other hand, attaining a high intensity modulation is necessary for achieving a high signal–noise ratio with the grating interferometry.⁷⁻⁹ Hence, for design optimization of x-ray grating interferometry, it is desirable to have a quantitative tool to predict if one can attain a good intensity modulation by using a given grating–detector distance along with a given x-ray spectrum.

To meet the need for a grating interferometer optimization, in this work we present a novel general theory that quantifies the diffraction orders in the interference fringes at any grating-to-detector distance. For the sake of generality, we assume the grating is a two-dimensional (2-D) phase grating of any phase shift value. The reason to study the 2-D phase grating interferometers is that from the 2-D grating formulas, we can straightforwardly derive the corresponding formulas for the 1-D grating interferometers through the dimensional reduction. In this work, we derive the Fourier coefficients of the interference intensity fringe for any given grating–detector distance, thereby providing a quantitative tool for grating

interferometry optimization. We organize the paper as follows. In Sec. 2, we briefly review the general theoretical formalism that underlines our new theory and discuss our strategy for the derivation. In Sec. 3, we present our results as follows. In Subsection 3.A.1, we present the formulas of the diffraction orders in the fringe patterns associated with a 2-D phase grating of any phase shift value. In Subsection 3.A.2, we present the corresponding formulas with a 1-D phase grating of any phase shift value. In Subsection 3.B, we apply our general formulas to polychromatic x-ray cases. We will introduce the concept of the visibility of a diffraction order and show how to use the visibility curve as a tool for interferometer geometry optimization. In Subsection 3.C, we apply our theory to design optimization of the so-called inverse geometry configuration. In the inverse geometry configuration, the phase grating is placed close to the source such that the magnification factor can be as high as a few tens. With such high magnification, the intensity fringes can be resolved directly by the imaging detector without using an additional absorbing grating. Consequently, this inverse geometry configuration will significantly reduce the radiation dose involved.¹⁹⁻²² We will show how the visibility curve is used in the optimization of inverse geometry configuration. We conclude the paper in Sec. 4.

2. MATERIALS AND METHODS

In this work, we investigate grating-based x-ray interferometers using a single phase grating. Figure 1 shows a general setup of such a single grating imaging with a point polychromatic x-ray source. In Fig. 1, S denotes a point source such as a microfocus x-ray tube, and G_1 depicts a 2-D checkerboard phase grating with a period of $p_1 = 2p$, as is shown in Fig. 2. The reason to consider a 2-D phase grating is that the 2-D phase grating interferometers have some advantages over the 1-D grating based systems. The 2-D phase grating

$\Delta\phi$	0	$\Delta\phi$	0	$\Delta\phi$	0	$\Delta\phi$	0
0	$\Delta\phi$	0	$\Delta\phi$	0	$\Delta\phi$	0	$\Delta\phi$
$\Delta\phi$	0	$\Delta\phi$	0	$\Delta\phi$	0	$\Delta\phi$	0
0	$\Delta\phi$	0	$\Delta\phi$	0	$\Delta\phi$	0	$\Delta\phi$
$\Delta\phi$	0	$\Delta\phi$	0	$\Delta\phi$	0	$\Delta\phi$	0
0	$\Delta\phi$	0	$\Delta\phi$	0	$\Delta\phi$	0	$\Delta\phi$
$\Delta\phi$	0	$\Delta\phi$	0	$\Delta\phi$	0	$\Delta\phi$	0
0	$\Delta\phi$	0	$\Delta\phi$	0	$\Delta\phi$	0	$\Delta\phi$

FIG. 2. A sample checkerboard phase grating.

interferometers are able to explore the multidirectional structures of samples and would enable us to develop more robust phase retrieval than that with the 1-D phase grating systems.^{20,22–26} Moreover, the formulas for the 1-D phase grating interferometry can easily be derived from the general two-dimensional theory through a dimension reduction. As is shown in Fig. 1, we denote the source-to-grating distance by R_1 and grating-to-detector distance by R_2 . In the setting we assume that the grating generates a phase shift of $\Delta\phi$ or 0, depending on the ray position. In practice, one often uses the so-called π -shift phase grating for its high diffraction efficiency. Note that for polychromatic x-ray, the grating-generated phase shift varies with the wavelength. If the grating generates a π -shift at the “central” wavelength λ_c , then the grating generates a phase shift $\Delta\phi = (\lambda/\lambda_c)\pi$ at a different wavelength λ in the spectrum. In this case, the phase shift $\Delta\phi$ could be greater or less than π , depending on the ratio λ/λ_c . In the setup shown in Fig. 1, the incident spherical x-ray wavefront is modulated by the grating with phase shifts and divided into tilted replicas. Through Fresnel diffraction from the grating to the detector downstream, these replicas mutually interfere and lead to intensity fringe patterns at the detector entrance. For monochromatic x-rays, the contrast of the fringe pattern will depend on the grating-to-detector distance. As is explained in the Introduction, for a given wavelength, the highly modulated self-images form only at the discrete fractional Talbot distances.^{4–18} In medical imaging, the polychromatic sources prevail. With a polychromatic x-ray beam, the intensity pattern is a sum of the intensities generated by each of the spectral components in the beam. Hence, with the polychromatic x-ray beam, there is no well-defined Talbot distances that would enable high-modulation intensity fringes. Rather, those Talbot distances get smeared out into patches, and the fringe modulation gets reduced. So far in the literature, there is no quantitative theory that is able to predict precisely the length of these patches and the associated fringe visibility with polychromatic x-rays. Since a high fringe visibility is required for achieving high signal–noise ratios in grating interferometry, it is desirable to be able to quantify the visibility of the fringe pattern at any distance behind the grating along with any x-ray spectrum. Equivalently, it is desirable to be able to quantify the visibility of the diffraction peaks, or the Fourier components of the intensity fringes. In this work, we set out to meet this need by deriving the formula of the Fourier coefficients of the intensity fringes.

We first study the intrinsic intensity fringes of the interferometry without a sample. We start to consider a phase grating system setup identical to Fig. 1 except replacing the source with a monochromatic point source of wavelength λ . The cases with polychromatic x-ray sources will be considered later. We assume that the grating is a two-dimensional checkerboard binary phase grating with a phase shift step of $\Delta\phi$ and a bidirectional period of $p_1 = 2p$ across the grating (Fig. 2), and we denote the transmission function of the grating by $G_1(\vec{r})$. As the incident spherical x-ray wavefront impedes upon the grating, the x-ray beam is modulated with the phase shift $\Delta\phi$ and divided into tilted replicas. The Fresnel diffraction of these replicas from the grating to the detector can be computed

accurately by using our wavefront evolution formula developed previously for the in-line phase-contrast imaging.^{27,28} In this framework of x-ray phase contrast imaging, we studied the phase space evolution of the Wigner distribution of the diffracted wavefront,²⁷ which we briefly review below. The reasons to use the Wigner distribution formalism are twofold. First, the Wigner distribution formalism inherently incorporates the partial spatial coherence of a wavefront into the theory. Second, Wigner distribution evolves in free space according to a very simple rule, so it facilitates the analysis of diffraction intensities.

The Wigner distribution $W(\vec{r}, \vec{u}; z)$ of a wavefront is defined as

$$W(\vec{r}, \vec{u}; z) = \int J(\vec{r} + \vec{q}/2, \vec{r} - \vec{q}/2; z) \cdot e^{-2\pi i \vec{q} \cdot \vec{u}} d\vec{q}, \quad (2)$$

where $J(\vec{r}_1, \vec{r}_2; z)$ is the mutual intensity of the wavefront at distance z from the source. The vector $\vec{u}$ denotes a coordinate vector of the two-dimensional Fourier space; hence, $\vec{u}$ is also called a spatial frequency vector. The mutual intensity specifies both the intensity and the coherence of x-ray wavefront.²⁹ Obviously, the Wigner distribution is defined in the 4D phase space $(\vec{r}, \vec{u})$ for a given distance z from the source plane. Moreover, the intensity of the wavefront at the detector plane is related to its Wigner distribution by

$$I(\vec{r}; R_1 + R_2) = \int W(\vec{r}, \vec{u}; R_1 + R_2) d\vec{u}. \quad (3)$$

During x-ray wave paraxial diffraction from the phase grating plane at $z = R_1$ to the entrance of imaging detector at $z = R_1 + R_2$, the Wigner distribution evolution is simply implemented by a phase space shearing³⁰

$$W(\vec{r}, \vec{u}; R_1 + R_2) = W(\vec{r} - \lambda R_2 \vec{u}, \vec{u}; R_1). \quad (4)$$

That is, when the wave propagates from $z = R_1$ to $z = R_1 + R_2$, the Wigner distribution at $z = R_1 + R_2$ can be found from the Wigner distribution at $z = R_1$ by replacing its argument $\vec{r}$ with $(\vec{r} - \lambda R_2 \vec{u})$. We call the displacement $\lambda R_2 \vec{u}$ as the phase space shearing length generated in the diffraction. The phase space shearing leads to wave superposition. We now consider the Fourier transform $\hat{I}(\vec{u}; R_1 + R_2)$ of the x-ray intensity at the detector plane ($z = R_1 + R_2$), which is defined as $\hat{I}(\vec{u}; R_1 + R_2) = \int I(\vec{r}; R_1 + R_2) \exp[-2\pi i \vec{r} \cdot \vec{u}] d\vec{r}$. Substituting Eqs. (3) and (4) into the integral and using the definition of Wigner distribution at $z = R_1$ in terms of the entrance wavefield and the phase grating transmission function $G_1(\vec{r})$, we find that $\hat{I}(\vec{u}; R_1 + R_2)$ is given by^{27,28}

$$\hat{I}(\vec{u}; R_1 + R_2) = I_{\text{in}} \int \mu_{\text{in}}(\vec{s} - \lambda R_2 \vec{u}/2, \vec{s} + \lambda R_2 \vec{u}/2) \cdot H(\vec{s}; \vec{u}) \cdot \exp(-2\pi i \vec{s} \cdot \vec{u}) d\vec{s}, \quad (5)$$

where

$$H(\vec{s}; \vec{u}) = G_1(\vec{s} - \lambda R_2 \vec{u}/2) \cdot G_1^*(\vec{s} + \lambda R_2 \vec{u}/2). \quad (6)$$

In this equation, the constant I_{in} denotes the incident x-ray intensity at the grating, and $\mu_{\text{in}}(\vec{s}_1, \vec{s}_2)$ denotes the complex degree of coherence of the x-ray illumination at the grating plane,²⁹ which depends on two position vectors $\vec{s}_1$ and $\vec{s}_2$,

defined by $\vec{s}_1 = \vec{s} - \lambda R_2 \vec{u}$ and $\vec{s}_2 = \vec{s} + \lambda R_2 \vec{u}$. Further simplifications of this equation depend on the nature of the x-ray sources. For a so-called Schell-model source, its complex degree of coherence $\mu_{in}(\vec{s}_1, \vec{s}_2)$ is spatially stationary such that

$$\mu_{in}(\vec{s}_1, \vec{s}_2) = \exp \left[i\pi \frac{\vec{s}_1^2 - \vec{s}_2^2}{\lambda R_1} \right] \cdot \tilde{\mu}_{in}(\vec{s}_1 - \vec{s}_2). \quad (7)$$

We call $\tilde{\mu}_{in}(\vec{s}_1 - \vec{s}_2)$ in above equation the reduced complex degree of coherence of the x-ray wavefield. Note that $\tilde{\mu}_{in}(\vec{s}_1 - \vec{s}_2)$ depends only on the difference $(\vec{s}_1 - \vec{s}_2)$.³⁰ The undulator sources in synchrotron facilities can often be treated as Schell-model sources. Moreover, although an anode source is a polychromatic x-ray source, for a given quasimonochromatic spectral component, the anode source is also a Schell-model source. This is because the complex degree of coherence $\mu_{in}(\vec{s}_1, \vec{s}_2)$ of an anode source can be determined by the van Cittert–Zernike theorem, and it satisfies Eq. (7).^{27,28} This being so, Eq. (5) can be simplified as^{27,28}

$$\hat{I}\left(\frac{\vec{u}}{M}\right) = I_{in} \cdot \tilde{\mu}_{in}\left(-\frac{\lambda R_2}{M} \vec{u}\right) \cdot \int H(\vec{s}; \vec{u}) \cdot \exp[-2\pi i \vec{s} \cdot \vec{u}] d\vec{s}, \quad (8)$$

where $\vec{u}$ denotes the spatial frequency vector at the grating plane. $M = (R_1 + R_2)/R_1$ is the geometric magnification, and H is defined in Eq. (6). In this equation, $\tilde{\mu}_{in}(-\lambda R_2 \vec{u}/M)$ accounts for the partially spatial coherence effect of the illuminating x-rays.

Equation (8) serves as the starting point for deriving the visibility of the diffraction orders behind a phase grating. In this work, we consider a point source, and for a spherical wavefront from the point source, its reduced complex degree of coherence is characterized by $\tilde{\mu}_{in}(-\lambda R_2 \vec{u}/M) = 1$. Note that there is a relative argument shift $\lambda R_2 \vec{u}/M$ in $H(\vec{r}; \vec{u})$, the cross-product of $G_1(\vec{r})$, and its complex conjugate $G_1^*(\vec{r})$. This shift in arguments $G_1(\vec{r})$ and $G_1^*(\vec{r})$ manifests the phase space shearing generated by the Fresnel diffraction, and we call this shift the phase space shearing length, denoted as $L(\vec{u}; \lambda) = \lambda R_2 \vec{u}/M$.^{27,28} In order to compute this integral, we note that the cross-product $G_1(\vec{s} + \lambda R_2/2M \vec{u}) \cdot G_1^*(\vec{s} - \lambda R_2/2M \vec{u})$ is again a two-dimensional array on the same periodic point-lattice as that of grating G_1 , so we can rewrite it as

$$H(\vec{s}; \vec{u}) = G_1(\vec{s} + L(\vec{u}; \lambda)/2) \cdot G_1^*(\vec{s} - L(\vec{u}; \lambda)/2) = 4p^2 C(\vec{s}; L(\vec{u}; \lambda)) \otimes \sum_{\vec{m} \in \mathbb{Z}^2} \delta^{(2)}(\vec{s} - 2p\vec{m}), \quad (9)$$

where $\vec{m} = (m, n)$ is a 2-D integer index, $\delta^{(2)}(\vec{s})$ denotes a two-dimensional Dirac function in the grating plane, and $\otimes$ represents the convolution operator. The assembly $\{\delta^{(2)}(\vec{s} - 2p\vec{m});$

$\vec{m} \in \mathbb{Z}^2\}$ describes a periodic point-lattice of period $p_1 = 2p$. In Eq. (9), $4p^2 C(\vec{s}; L(\vec{u}; \lambda))$ denotes the phase-shearing-generated unit cell that is attached to each of the two-dimensional lattice points such that the combined lattice represents the cross-product $G_1(\vec{s} + L(\vec{u}; \lambda)/2) \cdot G_1^*(\vec{s} - L(\vec{u}; \lambda)/2)$. From Eqs. (8) and (9), we can rewrite the Fourier transform of the x-ray irradiance as the following:

$$\begin{aligned} \hat{I}\left(\frac{\vec{u}}{M}; R_1 + R_2\right) &= I_{in} \cdot \hat{C}(\vec{u}; L(\vec{u}; \lambda)) \cdot \sum_{\vec{m} \in \mathbb{Z}^2} \delta^{(2)}\left(\vec{u} - \frac{\vec{m}}{2p}\right) \\ &= I_{in} \cdot \sum_{\vec{m} \in \mathbb{Z}^2} \hat{C}\left(\frac{\vec{m}}{2p}; L\left(\frac{\vec{m}}{2p}; \lambda\right)\right) \cdot \delta^{(2)}\left(\vec{u} - \frac{\vec{m}}{2p}\right), \end{aligned} \quad (10)$$

where $\hat{C}(\vec{u}; L(\vec{u}; \lambda))$ is the Fourier transform of $C(\vec{s}; L(\vec{u}; \lambda))$. Equation (10) dictates that the intensity at the detector plane is a superposition of fringes with discrete spatial frequencies $\{\vec{m}/2p; \vec{m} = (m, n) \in \mathbb{Z}^2\}$, each of which being also called a diffraction order. The Fourier coefficient of a diffraction order $\vec{m}/2p$ is given by $\hat{C}(\vec{m}/2p; L(\vec{m}/2p; \lambda))$. The lengthy derivation of the formulas for $\hat{C}(\vec{m}/2p; L(\vec{m}/2p; \lambda))$ is detailed in the Appendix. From Eq. (10), we can find the interference fringe pattern at the detector plane through an inverse Fourier transform

$$\begin{aligned} I(M\vec{r}; R_1 + R_2) &= \frac{I_{in}}{M^2} \\ &\cdot \sum_{\vec{m} \in \mathbb{Z}^2} \hat{C}\left(\frac{\vec{m}}{2p}; L\left(\frac{\vec{m}}{2p}; \lambda\right)\right) \cdot \exp\left[2\pi i \frac{\vec{m} \cdot \vec{r}}{2p}\right], \end{aligned} \quad (11)$$

where $I(M\vec{r}; R_1 + R_2)$ denotes the intensity fringe pattern at the detector plane with a SID of $R_1 + R_2$, $M\vec{r}$ is the position vector in detector plane, and $\vec{r}$ is the position vector on the phase grating plane. Once we find out the Fourier coefficients $\hat{C}(\vec{m}/2p; L(\vec{m}/2p; \lambda))$, we can compute the visibilities of the diffraction orders at any grating-to-detector distance for monochromatic and polychromatic x-rays.

3. RESULTS AND DISCUSSION

3.A. Diffraction orders in grating fringe pattern

3.A.1. Two-dimensional phase gratings

As is shown in Eq. (10), the intensity fringe of a phase grating interferometer comprises discrete diffraction orders, i.e., discrete spatial harmonics. Using the methods delineated in Sec. 2, through tedious calculation, we found the Fourier coefficient for any given diffraction order as follows:

$$\hat{C}\left(\frac{\vec{m}}{2p}; L\left(\frac{\vec{m}}{2p}; \lambda\right)\right) = \begin{cases} 1, & \text{if } m = n = 0, \\ 0, & \text{if } m + n = \text{odd}, \\ 2(1 - \cos \Delta \phi) \cdot f(k) \cdot f(l), & \text{if } m = 2k, n = 2l, \\ -\sin \Delta \phi \cdot \frac{\sin\left[\left(\frac{\pi \lambda R_2}{M p^2}\right) \cdot ((k + 1/2)^2 + (l + 1/2)^2)\right]}{\pi^2 (k + 1/2) \cdot (l + 1/2)}, & \text{if } m = 2k + 1, n = 2l + 1, \end{cases} \quad (12)$$

where

$$f(k) = (-1)^{\lfloor k\lambda R_2/Mp^2 \rfloor} \cdot \begin{cases} -\frac{1}{2}, & \text{if } k=0, \\ \frac{\sin\left(k^2\pi \frac{\lambda R_2}{Mp^2}\right)}{k\pi}, & \text{otherwise.} \end{cases} \quad (13)$$

In Eq. (13), symbol $\lfloor x \rfloor$ represents the largest integer number greater than x . So $(-1)^{\lfloor k\lambda R_2/Mp^2 \rfloor}$ swing between 1 and -1 as R_2 increases.

Equations (12) and (13) present the intensity fringe of a 2-D phase grating interferometer as a sum of discrete diffraction orders. The efforts in the Fourier analysis of intensity fringes with phase gratings can be traced back to earlier works in the optics literature.^{31–33} In these early works, the Fourier analysis was applied to the Fresnel field, or the diffracted wavefield. Specifically, the Fresnel field of the grating was expanded as $\psi(x, y) = \sum_{m,n \in \mathbb{Z}} A_{mn} \exp(i2\pi(mx + ny)/p_1)$, where A_{mn} are the functions of the grating-to-detector distance, x-ray wavelength, and grating's phase shift and its period p_1 .^{31–33} In these early works, the Fourier expansion of the fringe intensity is expressed as

$$I(x, y) = |\psi|^2 = \sum_{m,n,s,t \in \mathbb{Z}} A_{mn} A_{st}^* \cdot \exp\left\{2\pi i \frac{(m-s)x + (n-t)y}{p}\right\}. \quad (14)$$

However, this is only a formal expression for the intensity fringe pattern, no closed-form formulas of the intensity's Fourier coefficients were given,^{31–33} because in this approach, the calculation of any intensity's Fourier coefficient involves a summation of infinite series. In fact, for a given diffraction order (k, l) of the intensity, its Fourier coefficient is $C_{kl} = \sum_{m,n \in \mathbb{Z}} A_{m+k, n+l} A_{mn}^*$, where A_{mn}^* denotes the complex conjugate of A_{mn} . Hence, the Fourier coefficient C_{kl} is an infinite sum of all the terms $A_{m+k, n+l} A_{mn}^*$. It is usually hard to work out such summations for computation of the Fourier coefficients C_{kl} . Only at special grating-to-detector distances such as $R_2/M = p_1^2/2\lambda$, a relatively simple relationship between the intensity fringes and phase distribution of a 2-D phase grating can be derived.³² But the summation task becomes much more complicated at other distances, and no formula for Fourier coefficients of the intensity fringes at an arbitrary grating-to-detector distance had been established in these works.^{31–33} In contrast, in this work, our Fourier analysis is directly applied to the fringe intensity itself by using Eq. (11), and closed-form formulas of the intensity's Fourier coefficients are derived in Eqs. (12) and (13) as shown. Another advantage of our intensity-based Fourier analysis method is that it can be applied to grating interferometry with polychromatic x-ray sources through the integration of spectral components of the intensity. But the wavefield-based Fourier analysis method adopted in the early works^{31–33} will lose its rigor and utility with polychromatic sources since the fractional Talbot distances are wavelength-dependent and not well defined with polychromatic x-rays.

Several general features of Eqs. (11)–(13) are worth mentioning. The central peak (the zeroth-order peak), which represents the constant background intensity of the fringe, has an R_2 -independent Fourier coefficient of 1, as is expected from the energy conservation in diffraction. For all other diffraction orders, the Fourier coefficients $\hat{C}(\vec{m}/2p; L(\vec{m}/2p; \lambda))$ vary as oscillating sinusoidal functions of the distance R_2/M along the downstream direction, and the higher the order is, the smaller oscillation magnitude. For example, for odd diffraction orders $\vec{m} = (2k+1, 2l+1)$, the Fourier coefficients are proportional to $\sin[\pi(\lambda R_2/Mp^2) \cdot ((k+1/2)^2 + (l+1/2)^2)]$, as is listed in Eq. (12), so their periods (in terms of R_2/M) are order-dependent. The higher the order is, the smaller the period is, and the oscillation damps with increasing diffraction orders. The common (i.e., the largest) period among the odd diffraction orders is equal to $4p^2/\lambda = p_1^2/\lambda$. On the other hand, for the even diffraction orders $\vec{m} = (2k, 2l)$, the Fourier coefficients are proportional to $(-1)^{\lfloor k\lambda R_2/Mp^2 \rfloor + \lfloor l\lambda R_2/Mp^2 \rfloor} \cdot \sin(\pi k^2 \lambda R_2/Mp^2) \cdot \sin(\pi l^2 \lambda R_2/Mp^2)$, and we found that the common (the largest) period among all the even-orders is equal to $p^2/\lambda = p_1^2/4\lambda$, which is just a quarter of that for the odd diffraction orders. This periodicity in terms of R_2/M underlines the self-image phenomenon in the fractional Talbot distances. This periodicity analysis shows that the following distances behind the grating are the fractional Talbot distances of the 2-D phase gratings for parallel and cone-beam x-rays, respectively,

$$Z_{F-2D}(n_d) = n_d \cdot p_1^2/8\lambda, \quad (15)$$

$$R_2(n_d) = \frac{R_1 \cdot n_d \cdot p_1^2/8\lambda}{R_1 - n_d \cdot p_1^2/8\lambda}, \quad (16)$$

where $n_d > 0$ is an integer and p_1 is the grating's period. Moreover, by using Eqs. (11)–(13), we will be able to rigorously determine the fractional Talbot distances and the interference fringe patterns for two-dimensional checkerboard phase gratings. But in this paper, we concentrate on how to use Eqs. (11)–(13) to study the visibility of interference fringes at any given distance behind phase gratings.

3.A.2. One-dimensional phase gratings

While our theory so far deals with 2-D phase grating imaging, the theory can be straightforwardly extended to 1-D phase grating systems through dimensional reduction. In Eq. (12), dimensional reduction is carried out in the following way: for the even diffraction orders, change $f(k) \cdot f(l)$ in Eq. (12) to $f(k) \cdot f(0)$, because the grating varies only in one direction. With the same consideration, for the odd diffraction orders, change $-1/\pi^2$ to i/π and discard the term $(l+1/2)$. Then, we can derive the Fourier transform of the intensity fringes for 1-D phase gratings,

$$I(Mx; R_1 + R_2) = \frac{I_{in}}{M^2} \cdot \sum_{m \in \mathbb{Z}} \hat{C}\left(\frac{m}{2p}\right) \cdot \exp\left[2\pi i \frac{mx}{2p}\right], \quad (17)$$

where

$$\hat{C}\left(\frac{m}{2p}\right) = \begin{cases} 1, & \text{if } m = 0, \\ -(1 - \cos \Delta\phi) \cdot (-1)^{\lfloor k\lambda R_2/Mp^2 \rfloor} \cdot \frac{\sin\left(k^2\pi \frac{\lambda R_2}{Mp^2}\right)}{k\pi}, & \text{if } m = 2k, k \neq 0, \\ i \sin \Delta\phi \cdot \frac{\sin[\pi(\lambda R_2/Mp^2)(k+1/2)^2]}{(k+1/2)\pi}, & \text{if } m = 2k+1. \end{cases} \quad (18)$$

On the other hand, one can also directly compute $\hat{C}(m/2p)$ in Eq. (18) by literally following each of the derivation steps as is shown in the Appendix.

3.B. Visibilities of diffraction orders in intensity fringe patterns

The virtue of the derived formulas Eqs. (11)–(13) resides in their capability to predict how the diffraction orders in the intensity fringes evolve with the grating–detector distance. To see this, we define the visibility of a diffraction order as the ratio of its Fourier coefficient to that of the central peak. We denote the visibility of a diffraction order $(\vec{m}/2p)$ by $V(\vec{m}; \lambda; R_2)$, as it depends on the wavelength and the grating–detector distance as well. Since the Fourier coefficient of the central peak is always equal to 1, the visibility of a diffraction order is equal to its Fourier coefficient, $V(\vec{m}; \lambda; R_2) = \hat{C}(\vec{m}/2; L(\vec{m}/2p; \lambda))$. Note that $V(\vec{m}; \lambda; R_2)$ could be either positive or negative, and a change of its sign with grating–detector distance accounts for the phase reversal of the diffraction order during wave propagation. Intuitively, the visibility of a diffraction order reflects the contrast of this diffraction order, as compared to the central peak (the zeroth order). The higher the magnitude (in absolute value) of the visibility $V(\vec{m}; \lambda; R_2)$ for a diffraction order, the more prominent is this diffraction order. As is shown by Eqs. (12) and (13), the absolute value of the visibility $V(\vec{m}; \lambda; R_2)$ decreases with the increasing order number $\vec{m}$, reflecting the decreasing contrast with high diffraction orders. Fortunately, only the lowest diffraction orders are enough for phase retrieval. Moreover, with polychromatic x-rays, the formed intensity fringe is an incoherent sum of the intensity fringes generated by each of the spectral components. Consequently, the net Fourier coefficient of the diffraction order $\vec{m}/2p$ with polychromatic x-ray is equal to $\int S(\lambda) \hat{C}(\vec{m}/2; L(\vec{m}/2p; \lambda)) d\lambda$, where $S(\lambda)$ is the normalized x-ray fluence spectrum. Consequently, for polychromatic x-rays, the net visibility of the diffraction order $\vec{m}/2p$ is

$$V(\vec{m}; R_2) = \int S(\lambda) \hat{C}\left(\vec{m}/2; L\left(\frac{\vec{m}}{2p}; \lambda\right)\right) d\lambda. \quad (19)$$

To validate our results derived above, we compare them with numerical simulations. In the simulation, assuming a point polychromatic source, we compute the intensity fringes, $I_\lambda(\vec{r}; R_1 + R_2)$, for each of the wavelengths through numerical wave propagation. In the simulation the phase shifting with the grating is implemented by multiplication of the grating's transmission function, and the free space diffraction

is implemented by using the Fresnel diffraction propagator $W_\alpha = \exp[i\lambda R_2 |\vec{u}|^2/M]$ in the Fourier domain. The intensity fringe formed with a given wavelength is obtained as the square modulus of the calculated wavefront at the detector plane.

Once the intensity fringe for each wavelength λ is computed, the intensity of the polychromatic beam is the sum of all spectral components' intensities. The visibility, $V(\vec{m}; R_2)$, is then calculated by taking the computed intensity's Fourier transform valued at $\vec{m}/2p$. Repeating the computation with different R_2 , we then get a curve of the visibility varying with the grating–detector distance R_2 .

Figure 3 depicts how the diffraction order visibilities vary with increasing grating–detector distance R_2 . Figure 3 also

FIG. 3. The visibilities of the diffraction orders $[\vec{m} = (1, 1) \text{ and } (2, 0)]$ are plotted as a function of the grating-to-detector distance, assuming a 2-D checkerboard phase grating of $\pi/2$ -phase shift (at 20 keV) and a fixed source-to-grating distance $R_1 = 80$ cm. The curves are shown in two graphs and one for a given diffraction order. Each graph plots four curves corresponding to the results with both 20 keV and the 35 kVp x-ray beams for a given diffraction order, and the curves are computed with Eqs. (12) and (13), and with the Fresnel diffraction simulation, respectively. In the graphs, the labels $R_2(2)$, $R_2(6)$, and $R_2(10)$ denote the 2-D fractional Talbot distances for a $\pi/2$ -grating (at 20 keV). These graphs show that the visibility curves computed with Eqs. (12) and (13) are in good agreement with that from the numerical simulation.

compares the $V(\vec{m}; R_2)$ values computed by using Eqs. (12) and (13) with that obtained from a numerical Fresnel diffraction simulation. In the comparison, we assumed a point source operating at 35 kVp, with a tungsten target and a 50- μm rhodium filter. The x-ray spectrum of this beam is computed based on a validated tube spectrum model.³⁴ The average energy of this spectrum is 19.84 keV. The 2-D checkerboard phase grating was assumed to be a $\pi/2$ -grating of a 5- μm period for 20 keV x-ray, but its phase shift value varies with the wavelengths in the spectrum. The interferometer is assumed to have a fixed source-to-grating distance $R_1 = 80$ cm and an adjustable grating-detector distance R_2 . In Fig. 3, the visibilities of two diffraction orders, namely, $\vec{m} = (1,1)$ and $(2,0)$, are plotted separately in two graphs, and each graph plots four curves corresponding to the results with both 20 keV and the 35 kVp x-ray beams, obtained from the theory prediction and numerical simulation, respectively. In each graph, the abscissa refers to the grating-detector distance R_2 in meters. The labels $R_2(2)$, $R_2(6)$, and $R_2(10)$ denote the 2-D fractional Talbot distances for a $\pi/2$ -grating at 20 keV. These 2-D fractional Talbot distances are given by $R_2(4q+2) = (R_1 \cdot (4q+2) \cdot p_1^2/8\lambda) / (R_1 - (4q+2) \cdot p_1^2/8\lambda)$, as defined in Eqs. (15) and (16) with $n_d = 4q+2$ and $q = 0, 1, 2, \dots$. The ordinate refers to the visibility of a given diffraction order. For 20 keV x-rays, the visibility curve of the order $\vec{m} = (1,1)$ keeps oscillating between $\pm 4/\pi^2$ (± 0.405) and reaches its positive or negative peaks exactly at the fractional Talbot distances $\{R_2(4q+2)\}$ for $q = 0, 1, 2, \dots$. This suggests that the visibility of the order $\vec{m} = (1,1)$ can serve as an indicator of underlying fringe-intensity modulation. Note that the span of each of oscillation cycles increases with grating-detector distance, because the geometric magnification factor increases with grating-detector distance as well. On the other hand, the visibility curve of the order $\vec{m} = (2,0)$ oscillates with a lower magnitude between zero and $-1/\pi$ (-0.318). The visibility curves of the orders $(1,1)$ and $(2,0)$ oscillate out of sync with each other, as is predicted by Eq. (12). In addition, Fig. 3 shows the visibility curve for the order $\vec{m} = (1,1)$ with the 35 kVp polychromatic x-ray beam as is specified earlier. For this broadband x-ray beam, the visibility curves for the orders $(1,1)$ and $(2,0)$ oscillate with increasing grating-detector distance but with damped magnitudes, reflecting that the visibility peaks get broadened and smoothed. Note that the visibility for the order $(1,1)$ becomes diminished for very large grating-detector distances because of the broadband spectral averaging effects. Similar damping effects were observed and referred to as the panchromatic distance effect in the literature.²⁶ Figure 3 demonstrates that, for both the monochromatic (20 keV) and polychromatic x-rays, the visibility curves computed with Eqs. (12) and (13) are all in good agreement with that from the numerical simulation.

Therefore, Eqs. (11)–(13) present for the first time a theoretical tool for quantitatively analyzing the self-imaging phenomenon with polychromatic x-ray sources, and they can be valuable in the optimization of grating based imaging with monochromatic or polychromatic sources. Consider phase retrieval by using the Fourier spectrum analysis method.^{17–19} It is important to have high-contrast Fourier peaks of the intensity fringe for the extraction of the imaged object's phase

gradients. In the literature, the Fourier spectrum analysis of phase retrieval is only applied to the images acquired at the discrete fractional Talbot distances. With Eqs. (11)–(13), one can compute how the visibility of a diffraction order varies with the grating-to-detector distance R_2 . This predictive capability allows one to optimize the grating interferometer geometry without the constraints imposed by discrete fractional Talbot distances.

3.C. An example of the visibility analysis: The Inverse geometry setting

As one example, let us reconsider the design of a single grating imaging system with the inverse geometry configuration, which has been discussed in Sec. 1 earlier. In the inverse geometry setting, the phase grating is placed very much closer to the source than to the detector such that $R_2 \gg R_1$ and $M \gg 1$.^{20,21} The inverse geometry settings studied in the literature all impose the requirement of matching the fractional Talbot distance. In fact, for a monochromatic source and a given SID, the Talbot-distance matching requires that the grating-to-detector distance should satisfy the following constraint:²⁰

$$R_1 = \frac{\text{SID}}{2} \cdot \left(1 - \sqrt{1 - \frac{4Z_{F-2D}}{\text{SID}}} \right), \quad (20)$$

$$R_2 = \frac{\text{SID}}{2} \cdot \left(1 + \sqrt{1 - \frac{4Z_{F-2D}}{\text{SID}}} \right). \quad (21)$$

Obviously, Eqs. (20) and (21) show $R_2 > R_1$ in the inverse geometry. In contrast, most of x-ray grating interferometers developed so far adopt geometries with $R_2 < R_1$.^{6–15} In order to achieve high magnification factors, Eqs. (20) and (21) dictate that a large SID must be used for matching a fractional Talbot distance.^{20,21} For example, for a 20-keV x-ray interferometer based on a 2-D checkerboard phase grating of 5- μm period, in order to achieve a magnification factor of 15, Eqs. (20) and (21) dictate that the most compact geometry should set $R_1 = 10.8$ cm and $R_2 = 151.2$ cm, so SID = 1.62 m. For sake of convenience in discussion, let us call this geometry as interferometer-configuration #1. For clinical imaging application, a more compact configuration is desirable. Note that while configuration #1 satisfies the Talbot-distance matching equation [Eqs. (20) and (21)] for 20 keV x-rays, it will not match such Talbot-distance matching equations for a polychromatic beam with an average energy of 20 keV. As polychromatic sources prevail in clinical imaging, we wonder if one can configure a high-magnification grating interferometer with a shorter SID than configuration #1 and with comparable intensity modulation.

With guidance of Eqs. (12) and (13), we found that there are many options for high-magnification, single grating imaging with a reasonable SID of 1.3 m or shorter. Shown in Fig. 4 are the visibility curves for such a configuration, which uses the same phase grating as that in Fig. 3 but with a reduced source-to-grating distance $R_1 = 8.4$ cm. Note we purposely set R_1 so short such that there does not exist any grating-detector distance that matches any of the fractional Talbot distances for

FIG. 4. The visibility curves of the two diffraction orders [$\vec{m} = (1,1)$ and $(2,0)$] are replotted for the system settings with reduced source-to-grating distance $R_1 = 8.4$ cm and with otherwise identical parameters as in Fig. 3. The short source-to-grating distance R_1 rules out the matching of any fractional Talbot distances at 20 keV. Note that the visibility curve of the order $\vec{m} = (1,1)$ does not oscillate with increasing grating-to-detector distance any more. The visibility of the order $(1,1)$ increases first monotonically in its magnitude with increasing grating–detector distance and then starts to plateau out with increasing grating–detector plane distance. These replotted graphs show again that the visibility curves computed with Eqs. (12) and (13) are in good agreement with that from the numerical simulation.

20 keV x-rays. In other words, with $R_1 = 8.4$ cm, Eqs. (20) and (21) have no solution at all for 20 keV x-ray. In Fig. 4, the visibilities of two orders $(1,1)$ and $(2,0)$ are plotted separately in two graphs, on each for the two diffraction orders. These curves were obtained by using two methods, the direct computation based on Eqs. (12) and (13) and the numerical Fresnel diffraction simulation, respectively. The curves in Fig. 4 correspond to the results for 20 keV and the 35 kVp x-ray beams, respectively. As is shown in Fig. 4, all the visibility curves computed using our formulas Eqs. (12) and (13) are all in good agreement with the curves computed with the Fresnel diffraction simulation. There are several interesting features of Fig. 4 that are worth mentioning. First, different from the visibility curves in Fig. 3, the visibility curves of the order $\vec{m} = (1,1)$ in Fig. 4 do not oscillate with increasing grating-to-detector distance, unlike before. The visibility for the order $(1,1)$ increases first monotonically in its magnitude with increasing grating–detector distance and then starts to plateau out with increasing grating–detector distance. Second, in spite of this mismatch with Talbot distances, our theory predicts that one can still achieve a high-magnitude visibility for the $(1,1)$ -order as long as the grating–detector distance $R_2 > 0.5$ m, regardless of using either monochromatic or polychromatic

x-rays. For example, for the 35 kVp x-ray beam as specified earlier, the visibility plateau approaches to -0.354 for the $(1,1)$ -order. On the other hand, the magnitude of visibility for order $(2,0)$ peaks only at a short grating–detector distance and then decreases with increasing grating–detector distance, as is shown in Fig. 4.

Based on the visibility curves presented in Fig. 4, we can design a single grating interferometer with a more compact high-magnification configuration by removing the constraint of the Talbot-distance matching. To select a grating–detector distance for the system, we have imposed following requirements: (i) the main diffraction order should have a large-magnitude visibility at the selected grating–detector distance; (ii) the system detector can readily resolve the interference fringe pattern at this distance; (iii) the size of the resulting system should be as compact as feasible. The system in design consists of a grating with $\pi/2$ -phase shift at 20-keV, a micro-focus tube, which is with tungsten target and a rhodium filter and operating at 35 kVp as is specified above, and a detector with its pixel pitch $p_D = 25$ μm . We set the source-to-grating distance $R_1 = 8.4$ cm, the same as is studied in Fig. 4. Under the guidance of Fig. 4, we set the grating–detector distance to $R_2 = 117.6$ cm. We call this setting as the interferometer-configuration #2. Note that in this configuration R_1 is set so short such that there does not exist any grating–detector distance that matches any of the fractional Talbot distances for 20 keV x-rays. At this grating–detector distance, Fig. 4 shows that the magnitude of the $(1,1)$ -order’s visibility is as high as 0.354. Since the resulting geometric magnification factor M is 15, one period of the intensity fringe pattern will include three detector pixels. In this setting, the resulting system SID is equal to 1.26 m, a more compact size.

To compare the intensity fringes generated with the interferometer-configurations #1 and #2, we simulated the interference patterns based on the Fresnel diffraction of the 35 kVp beam for the two settings. Figures 5(a) and 5(b) depict the interference fringe patterns obtained from the numerical simulation for these two settings. Figure 5(a) shows the fringe pattern obtained by using the Talbot-distance matching configuration #1, and Fig. 5(b) shows the intensity fringe with the configuration #2. The two intensity fringe patterns are hardly distinguishable. To measure the subtle differences in the intensity modulation, we adopt the intensity-visibility commonly defined as $V_I = (I_{\max} - I_{\min}) / (I_{\max} + I_{\min})$. We found that the intensity fringe with the configuration #1 [Fig. 5(a)] has a good intensity-visibility of 0.680, while the intensity fringe with configuration #2 has a comparably good intensity-visibility of 0.644. This high intensity-visibility demonstrates that this configuration #2 is able to provide a high intensity modulation while ensuring a more compact size as compared to the Talbot-distance matching configuration #1. Figure 5(c) shows the Fourier spectrum of the fringe pattern in Fig. 5(b). The gray scale depicts the magnitude of the visibility of a diffraction order. In Fig. 5(c), the central peak has a visibility of 1. The four peaks marked by 1 represent the four diffraction orders $\vec{m} = (\pm 1, \pm 1)$, and each of the peaks has a visibility-magnitude of 0.354. These visibility values are in good agreement with that predicted by Eqs. (12) and (13).

FIG. 5. Intensity interference fringe pattern obtained from the numerical simulation. (a) Intensity fringe pattern obtained by using the Talbot-distance matching interferometer-configuration #1. The fringe patterns has a good intensity-visibility = 0.680. (b) Intensity fringe with the interferometer-configuration #2. The intensity fringe has a comparably good intensity-visibility of 0.644. (c) Fourier spectrum of the fringe pattern in Fig. 5(b). The central peak has a visibility of 1. The four peaks marked by 1 represent the four diffraction orders, each of the peaks has a visibility-magnitude of 0.354. These visibility values are in good agreement with that predicted by Eqs. (12) and (13).

In order to further validate the system design discussed above, we performed a numerical simulation of phase retrieval with a numerical phantom. The simulated system includes a grating of $\pi/2$ -phase shift at 20-keV, a microfocus tube with W/Rh target/filter and 35-kVp tube voltage, and a detector with $25\mu\text{m}$ -pixels. The system geometry setting is the same as the configuration #2 discussed earlier, which employs a source-to-grating distance of 8.4 cm and a grating–detector distance of 117.6 cm. A numerical tissue phantom was set relatively close to the detector such that the phantom is projected with a magnification factor of 2. The numerical phantom consists of 5-cm block of breast adipose tissue with a sphere-like glandular tissue lump of 1.5 mm in size inside the tissue block. The elemental compositions of the breast adipose and glandular tissues are obtained from the measurement results from the literature.^{35,36} Based on these tissues' elemental compositions, the mass attenuation coefficients for each of photon

energies and electron densities are determined from a standard literature.³⁷ A ray-tracing algorithm was used to compute the ray integrals of the tissue linear attenuation coefficients and tissue electron densities for each of photon energies in the x-ray spectrum. The x-rays undergo phase shift and attenuation through the phantom, and thereby, the optical transmission function of the phantom was determined by using the ray integrals of the tissue linear attenuation coefficients and electron densities. In this simulation, the intensity fringe pattern was obtained by numerical wave propagation, as described in details in Sec. 3.B. The intensity pattern was computed and rebinned over each of the $25\mu\text{m}$ -pixels. The phase retrieval is implemented by using the Fourier spectrum analysis which requires only a single exposure, different from the phase stepping method that needs multiple exposures.^{6–9,17–19} The single-exposure based phase retrieval would allow radiation dose reduction and facilitated image acquisition.

FIG. 6. Retrieved phase gradient map of a numerical phantom imaged with interferometer-configuration #2. (a) Retrieved map of the phantom's phase gradient in the forward diagonal direction, which is the phantom's phase map. The map is retrieved from through the Fourier spectrum analysis of the (1,1)-peak. (b) Retrieved map of the phantom's phase gradient in the backward diagonal direction. It is retrieved through the Fourier spectrum analysis of the (1,−1)-peak. (c) Red curve shows the profile of the retrieved phase gradient, as compared to the blue curve of the true phase gradients. The profiles are drawn along a horizontal trace passing the lump's center.

In the phase retrieval, the rebinned intensity fringes were Fourier transformed, and the (1,1) and (1,-1)-peaks in the spatial frequency spectrum were analyzed according to the standard Fourier spectrum method of phase retrieval.¹⁶⁻¹⁹ Briefly speaking, phase retrieval involves shifting the two peaks to the origin of the Fourier domain, subsequent inverse-Fourier transformation, and then argument-extraction. Interested readers are referred to Refs. 17 and 19 for details of the method. The Fourier spectrum analysis of the (1,1)-peak as outlined above gives a map of the phantom's phase gradient $(\partial_x + \partial_y)\Phi$. Figure 6(a) shows the retrieved map of the phase gradient $(\partial_x + \partial_y)\Phi$ along the forward diagonal direction, where $\Phi(\vec{r})$ is the phantom's phase map. Shown in Fig. 6(b) is the retrieved map of the phantom's phase gradient $(\partial_x - \partial_y)\Phi$ along the backward diagonal direction, as retrieved through the Fourier spectrum analysis of the (1,-1)-peak. The high visibilities of the $(\pm 1, \pm 1)$ -orders in configuration #2 make them good carrier signals to encode the phantom's information for enabling robust phase retrieval. In Fig. 6(c), the red curve shows the profile of the retrieved phase gradient, as compared to the blue curve representing the true phase gradients. The profiles are drawn along a horizontal trace passing the lump's center. The errors of the retrieved phase gradient values, as compared to the true value, are within 6.9%. These errors are attributable to beam hardening effects and to errors with the numerical simulation, which deserves further study. Furthermore, the different edge enhancement patterns presented in Figs. 6(a) and 6(b) demonstrate that it is advantageous to use a 2-D phase grating system rather than a 1-D grating system for the samples with multidirectional structures. Moreover, a 2-D phase grating system can provide more robust phase maps than a 1-D grating system does.^{20,24-26} Detailed discussion on this aspect is out of the scope of this work.

4. DISCUSSION AND CONCLUSIONS

In this work, we present a novel theory of Talbot interferometry. This theory presents a general theoretical formalism of Talbot interferometry that is valid for any phase shift value of the grating and for either monochromatic or polychromatic x-ray sources. Our theory, as is instilled in Eqs. (11)–(13), provides a tool to study the interference fringe patterns not only at the fractional Talbot distances but also at any position behind the phase grating. This theory will be especially useful in future medical applications of x-ray Talbot interferometry. In medical imaging, polychromatic anode sources prevail, so the concept of the Talbot self-image distance itself is not well defined for polychromatic x-ray, because both the grating phase shift and Talbot distances are x-ray wavelength-dependent. So far there is no quantitative theory that is able to predict if good intensity modulation would be attainable at a given grating-to-detector distance for a given x-ray spectrum, as high intensity modulation is required for achieving high signal-noise ratios in grating imaging.⁶⁻⁹ To meet these needs, we propose to compute the visibilities $V(\vec{m}; R_2)$ of diffraction orders. Equations (11)–(13) lay out the theoretical foundation to compute the visibility $V(\vec{m}; R_2)$ as a function of the grating-to-detector distance and x-ray spectral contents. The

net visibilities $V(\vec{m}; R_2)$ for a given x-ray spectrum can serve as the indicators of underlying fringe-intensity modulation. The high visibility of a diffraction order makes it a good carrier signal to encode the sample's information for robust phase retrieval, as is demonstrated in Sec. 3.B. Of course, a detailed signal-noise analysis is out of the scope of this paper. Hence, enabling computation of the visibility of any diffraction order for any polychromatic x-ray spectrum, our theory provides a quantitative design optimization tool for x-ray grating-based differential phase contrast imaging.

In the discussions throughout this work, we assume that the source is a microfocus source simulating a point x-ray source. Under this assumption, the reduced complex degree of coherence, e.g., $\tilde{\mu}_{in}(-\lambda R_2 \vec{u}/M)$ in Eq. (8), is equal to 1 for any diffraction order and any grating-detector distance. In practice, for an x-ray tube of finite focal spot, a source grating should be installed near the source to break the source into an array of small virtual sources, and the resulting interferometer is usually called the Talbot-Lau interferometer in the literature.^{3,4,8,9} The theory developed in this work can still be applied to Talbot-Lau interferometers, provided that the Fourier coefficients of all diffraction order are modified from $\hat{C}(\vec{m}/2p; L(\vec{m}/2p; \lambda))$ to the product $\tilde{\mu}_{in}(-\lambda R_2 \vec{u}/M) \cdot \hat{C}(\vec{m}/2p; L(\vec{m}/2p; \lambda))$. Using the Van Cittert-Zernike theorem, $\tilde{\mu}_{in}(-\lambda R_2 \vec{u}/M)$ is just a rescaled Fourier transform of the transmission function of the source grating.^{27,28} With a source grating the modulus of $\tilde{\mu}_{in}(-\lambda R_2 \vec{u}/M)$ is generally less than 1, and it decreases with increasing $\vec{m}$ and increasing grating-detector distance. Hence, the magnitude of the visibility of a diffraction order will be reduced by a factor of the modulus of $\tilde{\mu}_{in}(-\lambda R_2 \vec{u}/M)$, as compared to the point source cases.²⁸

In conclusion, in this work we developed a novel theory of the interference fringes in phase grating x-ray interferometry. In this theory, the Fourier coefficients of the interference intensity fringe are derived for an arbitrary grating-detector distance. This theory determines the visibility of any diffraction order as a function of the grating-to-detector distance, the phase shift of the grating, and the x-ray spectrum. We demonstrate that the visibilities of diffraction orders can serve as the indicators of the underlying interference intensity modulation. Applying the theory to conventional and the inverse geometry configurations of single-grating interferometers, we demonstrated that the proposed theory provides a quantitative tool for the interferometer optimization with or without the Talbot-distance constraints. The theory developed in this work provides a quantitative tool in design optimization of the phase grating x-ray interferometers.

ACKNOWLEDGMENTS

The authors gratefully acknowledge the support of the NIH Grant Nos. 1R01CA142587 and R01CA193378. Hong Liu would like to acknowledge as well a grant from the University of Oklahoma Charles and Peggy Stephenson Cancer Center funded by the Oklahoma Tobacco Settlement Endowment Trust, and the support of the Charles and Jean Smith Chair

endowment fund. The authors thank Gretchen Raterman for her help in editing the paper.

APPENDIX: THE DERIVATION OF DIFFRACTION ORDER $\hat{C}(\vec{m}/2p; L(\vec{m}/2p; \lambda))$

The appendix that we present here is to discuss the details of the derivation of Eq. (12).

Let G_1 be the two-dimensional checkerboard binary phase grating with a phase shift step of $\Delta\phi$ and a bidirectional period of $p_1 = 2p$ across the grating. Then, G_1 can be expressed mathematically to $G_1(\vec{r}) = \exp[i\Delta\phi \cdot h(\vec{r})]$, where $\vec{r} = (x_1, x_2)$ is the position vector in grating plane, and

$$h(\vec{r}) = \begin{cases} 1, & \text{if } \vec{r}_0 \in \left[-\frac{1}{2}, 0\right)^2 \cup \left[0, \frac{1}{2}\right)^2, \\ 0, & \text{otherwise,} \end{cases} \quad (\text{A1})$$

where $\vec{r}_0 = (\text{Rem}(x_1/2p) - 1/2, \text{Rem}(x_2/2p) - 1/2)$, $\text{Rem}(a) = a - [a]$, $[a]$ represents the largest integer number greater than a , and $[a, b]^2$ denotes the two-dimensional rectangular region $[a, b] \times [a, b]$ that does not include the top and right boundaries. For $\vec{r} = (x_1, x_2)$, $\vec{u} = (u_1, u_2)$, let

$$Q(\vec{r}; \vec{u}) = H(\vec{r} + \frac{\lambda R_2}{2M} \vec{u}; \vec{u}), \quad (\text{A2})$$

where $H(\vec{r}; \vec{u})$ is defined in Eq. (6). Since $Q(\vec{r}; \vec{u})$ is periodic, with respect to $\vec{r}$, of $p_1 = 2p$, we can write

$$Q(\vec{r}; \vec{u}) = Q_0(\vec{r}; \vec{u}) \otimes \sum_{\vec{m} \in \mathbb{Z}^2} \delta^{(2)}(\vec{r} - 2p\vec{m}), \quad (\text{A3})$$

where $\otimes$ is the convolution operator, and

$$Q_0(\vec{r}; \vec{u}) = \begin{cases} \exp\left[-i\Delta\phi \left(h\left(\vec{r} + \frac{\lambda R_2}{M} \vec{u}\right) - h(\vec{r})\right)\right], & \text{if } \vec{r} \in [-p, p]^2; \\ 0, & \text{otherwise.} \end{cases} \quad (\text{A4})$$

Then by Poisson summation formula,

$$\hat{Q}(\vec{v}; \vec{u}) = \frac{1}{4p^2} \hat{Q}_0(\vec{v}; \vec{u}) \cdot \sum_{\vec{m} \in \mathbb{Z}^2} \delta^{(2)}\left(\vec{v} - \frac{\vec{m}}{2p}\right). \quad (\text{A5})$$

	-p	-b1	0	p-b1	p
-p	1	0	0	1	
-b2	0	1	1	0	
0	0	1	1	0	
p-b2	1	0	0	1	
p					

(a)

	-p	-b1	0	p-b1	p
-p	0	1	1	0	
-b2	1	0	0	1	
0	1	0	0	1	
-b2	0	1	1	0	
-p					

(b)

	-p	-b1	0	p-b1	p
-p	1	1	0	0	
-b2	1	1	0	0	
0	0	0	1	1	
-b2	0	0	1	1	
-p					

(c)

FIG. 7. Values of function h for $\vec{r} \in (-p, p) \times (-p, p)$. (a) $h(\vec{r} + (\lambda R_2/M)\vec{u})$ when $n_1 + n_2$ is even. (b) $h(\vec{r} + (\lambda R_2/M)\vec{u})$ when $n_1 + n_2$ is odd. (c) $h(\vec{r})$.

Thus, Eq. (8) leads to

$$\begin{aligned} \hat{I}\left(\frac{\vec{u}}{M}; R_1 + R_2\right) &= I_{\text{in}} \cdot \hat{H}(\vec{u}; \vec{u}) = I_{\text{in}} \cdot \frac{1}{4p^2} \exp\left[-\pi i \frac{\lambda R_2}{M} \vec{u} \cdot \vec{u}\right] \\ &\quad \cdot \hat{Q}_0(\vec{u}; \vec{u}) \cdot \sum_{\vec{m} \in \mathbb{Z}^2} \delta^{(2)}\left(\vec{u} - \frac{\vec{m}}{2p}\right) \\ &= I_{\text{in}} \cdot \frac{1}{4p^2} \sum_{\vec{m} \in \mathbb{Z}^2} \exp\left[-\pi i \frac{\lambda R_2}{4Mp^2} |\vec{m}|^2\right] \\ &\quad \cdot \hat{Q}_0\left(\frac{\vec{m}}{2p}; \frac{\vec{m}}{2p}\right) \cdot \delta^{(2)}\left(\vec{u} - \frac{\vec{m}}{2p}\right), \end{aligned} \quad (\text{A6})$$

since $\delta^{(2)}(\vec{u} - \vec{m}/2p) = 0$ when $\vec{u} \neq \vec{m}/2p$. Compare to Eq. (10), we only need to show

$$\begin{aligned} \hat{Q}_0\left(\frac{\vec{m}}{2p}; \frac{\vec{m}}{2p}\right) &= 4p^2 \exp\left[\pi i \frac{\lambda R_2}{4Mp^2} |\vec{m}|^2\right] \\ &\quad \cdot \hat{C}\left(\frac{\vec{m}}{2p}; L\left(\frac{\vec{m}}{2p}; \lambda\right)\right), \end{aligned} \quad (\text{A7})$$

where $\hat{C}(\vec{m}/2p; L(\vec{m}/2p; \lambda))$ satisfies Eqs. (12) and (13).

Now, denoting $n_k = \lfloor \lambda R_2 u_k / Mp \rfloor$, and $b_k = p \cdot \text{Rem}(\lambda R_2 u_k / Mp)$, $k = 1, 2$, it is easy to see $h(\vec{r} + \lambda R_2 / M \cdot \vec{u})$ and $h(\vec{r})$ have values shown in Fig. 7. Thus for $\vec{v} = (v_1, v_2)$, we get, by directly computing the integral,

$$\hat{Q}_0(\vec{v}; \vec{u}) = -\frac{1}{4\pi^2 v_1 v_2} \begin{cases} K_1 \cdot J_1 + K_2 \cdot J_2, & \text{if } n_1 + n_2 = \text{odd}, \\ K_1 \cdot J_2 + K_2 \cdot J_1, & \text{if } n_1 + n_2 = \text{even}, \end{cases} \quad (\text{A8})$$

where

$$K_1 = (1 + B_1^*)(1 + B_2^*), \quad (\text{A9})$$

$$K_2 = C_g^*(1 + B_1^* B_2^*) + C_g(B_1^* + B_2^*), \quad (\text{A10})$$

$$J_1 = (1 - A_1)(A_2 - B_2) + (A_1 - B_1)(1 - A_2), \quad (\text{A11})$$

$$J_2 = (A_1 - B_1)(A_2 - B_2) + (1 - A_1)(1 - A_2), \quad (\text{A12})$$

$A_k = \exp[2\pi i b_k v_k]$, $B_k = \exp[2\pi i p v_k]$, $k = 1, 2$, and $C_g = \exp[-i\Delta\phi]$.

By taking the limit of $\hat{Q}_0(\vec{v}; \vec{u})$ (letting $\vec{v}, \vec{u}$ go to $(0, 0)$, $(0, n/2p)$, $(m/2p, 0)$, and $(m/2p, n/2p)$, respectively), Eq. (A7) can be easily confirmed.

By changing the 2-D checkerboard phase grating to 1-D grating, using the same way above (replacing the 2-D integral to 1-D), one can easily derive Eqs. (17) and (18) directly.

- ^{a1}Authors to whom correspondence should be addressed. Electronic addresses: xwu@uabmc.edu and liu@ou.edu
- ¹A. Snigirev *et al.*, "On the possibilities of x-ray phase contrast micro-imaging by coherent high-energy synchrotron radiation," *Rev. Sci. Instrum.* **66**, 5486–5492 (1995).
 - ²S. Wilkins, T. Gureyev, D. Gao, A. Pogany, and A. Stevenson, "Phase contrast imaging using polychromatic hard x-ray," *Nature* **384**, 335–338 (1996).
 - ³K. A. Nugent, "Coherent methods in the x-ray sciences," *Adv. Phys.* **59**, 1–99 (2010).
 - ⁴A. Bravin, P. Coan, and P. Suortti, "X-ray phase-contrast imaging: From pre-clinical applications towards clinics," *Phys. Med. Biol.* **58**, R1–R35 (2013).
 - ⁵P. Cloetens, J. P. Guigay, C. De Martino, J. Baruchel, and M. Schlenker, "Fractional Talbot imaging of phase gratings with hard x-rays," *Opt. Lett.* **22**, 1059–1061 (1997).
 - ⁶A. Momose, S. Kawamoto, I. Koyama, Y. Hamaishi, H. Takai, and Y. Suzuki, "Demonstration of x-ray Talbot interferometry," *Jpn. J. Appl. Phys., Part 2* **42**, L866–L868 (2003).
 - ⁷T. Weitkamp, A. Diaz, C. David, F. Pfeiffer, M. Stampanoni, P. Cloetens, and E. Ziegler, "X-ray phase imaging with a grating interferometer," *Opt. Express* **13**, 6296–6304 (2005).
 - ⁸A. Momose, "Recent advances in x-ray phase imaging," *Jpn. J. Appl. Phys., Part 1* **44**, 6355–6367 (2005).
 - ⁹F. Pfeiffer, T. Weitkamp, O. Bunk, and C. David, "Phase retrieval and differential phase-contrast imaging with low-brilliance x-ray sources," *Nat. Phys.* **2**, 258–261 (2006).
 - ¹⁰Z. T. Wang, K. J. Kang, Z. F. Huang, and Z. Q. Chen, "Quantitative grating-based x-ray dark-field computed tomography," *Appl. Phys. Lett.* **95**, 094105 (2009).
 - ¹¹W. Yashiro, Y. Terui, K. Kawabata, and A. Momose, "On the origin of visibility contrast in x-ray Talbot interferometry," *Opt. Express* **18**, 16890–16901 (2010).
 - ¹²P. P. Zhu, K. Zhang, Z. L. Wang, Y. J. Liu, X. S. Liu, Z. Y. Wu, S. A. McDonald, F. Marone, and M. Stampanoni, "Low-dose, simple, and fast grating-based x-ray phase-contrast imaging," *Proc. Natl. Acad. Sci. U. S. A.* **107**, 13576–13581 (2010).
 - ¹³G. H. Chen, N. Bevins, J. Zambelli, and Z. Qi, "Small-angle scattering computed tomography (SAS-CT) using a Talbot-Lau interferometer and a rotating anode x-ray tube: Theory and experiments," *Opt. Express* **18**, 12960–12970 (2010).
 - ¹⁴X. Tang, Y. Yang, and S. Tang, "Characterization 865 of imaging performance in differential phase contrast CT compared with the conventional CT – Noise power spectrum nps(k)," *Med. Phys.* **38**, 4386–4395 (2011).
 - ¹⁵N. Bevins, J. Zambelli, K. Li, Z. Qi, and G.-H. Chen, "Multicontrast x-ray computed tomography imaging using Talbot-Lau interferometry without phase stepping," *Med. Phys.* **39**, 424–428 (2012).
 - ¹⁶X. Tang, Y. Yang, and S. Tang, "Characterization of imaging performance in differential phase contrast CT compared with the conventional CT: Spectrum of noise equivalent quanta NEQ(k)," *Med. Phys.* **39**, 4467–4482 (2012).
 - ¹⁷M. Takeda, H. Ina, and S. Kobayashi, "Fourier-transform method of fringe-pattern analysis for computer-based topography and interferometry," *J. Opt. Soc. Am.* **72**, 156–160 (1982).
 - ¹⁸H. Wen, E. Bennett, M. Hegedus, and S. Carroll, "Spatial harmonic imaging of x-ray scattering—Initial results," *IEEE Trans. Med. Imaging* **27**, 997–1002 (2008).
 - ¹⁹E. Bennett, R. Kopace, A. Stein, and H. Wen, "A grating-based single shot x-ray phase contrast and diffraction method for *in vivo* imaging," *Med. Phys.* **37**, 6047–6054 (2010).
 - ²⁰A. Momose, H. Kuwabara, and W. Yashiro, "X-ray phase imaging using Lau effects," *Appl. Phys. Express* **4**, 066603 (2011).
 - ²¹N. Morimoto, S. Fujino, K. Ohshima, J. Harada, T. Hosoi, H. Watanabe, and T. Shimura, "X-ray phase contrast imaging by compact Talbot-Lau interferometer with a single transmission grating," *Opt. Lett.* **39**, 4297–4300 (2014).
 - ²²M. Jiang, C. Wyatt, and G. Wang, "X-ray phase-contrast imaging with three 2D gratings," *Int. J. Biomed. Imaging* **2008**, 827152.
 - ²³J. Rizzi, T. Weitkamp, N. Guérineau, M. Idir, P. Mercere, G. Druart, G. Vincent, P. Silva, and J. Primot, "Quadriwave lateral shearing interferometry in an achromatic and continuously self-imaging regime for future x-ray phase imaging," *Opt. Lett.* **36**, 1398–1400 (2011).
 - ²⁴G. Sato, T. Kondoh, H. Itoh, S. Handa, K. Yamaguchi, T. Nakamura, K. Nagai, C. Ouchi, T. Teshima, Y. Setomoto, and T. Den, "Two-dimensional gratings-based phase-contrast imaging using a conventional x-ray tube," *Opt. Lett.* **36**, 3551–3553 (2011).
 - ²⁵H. Itoh, K. Nagai, G. Sato, K. Yamaguchi, T. Nakamura, T. Kondoh, C. Ouchi, T. Teshima, Y. Setomoto, and T. Den, "Two-dimensional grating-based x-ray phase-contrast imaging using Fourier transform phase retrieval," *Opt. Express* **19**, 3339–3346 (2011).
 - ²⁶J. Rizzi, P. Mercere, M. Idir, P. Da Silva, G. Vincent, and J. Primot, "X-ray phase contrast imaging and noise evaluation using a single phase grating interferometer," *Opt. Express* **21**, 17340–17351 (2013).
 - ²⁷X. Wu and H. Liu, "A new theory of phase-contrast x-ray imaging based on Wigner distributions," *Med. Phys.* **31**, 2378–2384 (2004).
 - ²⁸X. Wu and H. Liu, "Phase-space evolution of x-ray coherence in phase-sensitive imaging," *Appl. Opt.* **47**, E44–E52 (2008).
 - ²⁹J. Goodman, *Statistical Optics* (John Wiley & Sons, Inc., New York, 1985).
 - ³⁰L. Mandel and E. Wolf, *Optical Coherence and Quantum Optics* (Cambridge University Press, Cambridge, 1995).
 - ³¹J. M. Cowley and A. F. Moodie, "Fourier images i: The point source," *Proc. Phys. Soc., London, Sect. B* **70**(5), 486–496 (1957).
 - ³²J. M. Cowley and A. F. Moodie, "Fourier images iv: The phase grating," *Proc. Phys. Soc., London* **76**(3), 378–384 (1960).
 - ³³J. T. Winthrop and C. R. Worthington, "Theory of fresnel images. i. Plane periodic objects in monochromatic light," *J. Opt. Soc. Am.* **55**, 373–381 (1965).
 - ³⁴D. Tucker, G. Barnes, and X. Wu, "Molybdenum target x-ray spectra: A semi-empirical model," *Med. Phys.* **18**, 402–407 (1991).
 - ³⁵G. Hammerstein, D. Miller, D. White, J. Laughlin, M. Masterson, and H. Woodard, "Absorbed radiation dose in mammography," *Radiology* **130**, 485–491 (1979).
 - ³⁶X. Wu, A. Yan, and H. Liu, "X-ray phase-shifts-based method of volumetric breast density measurement," *Med. Phys.* **39**, 4239–4244 (2012).
 - ³⁷X-Ray Mass Attenuation Coefficients, URL <http://www.fermentas.com/techinfo/nucleicacids/maplambda.htm>.