Phase retrieval in quantitative x-ray microtomography with a single sample-to-detector distance

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Phase retrieval extracts quantitative phase information from x-ray propagation-based phase-contrast images. Notwithstanding inherent approximations, phase retrieval using a single sample-to-detector distance (SDD) is very attractive, because it imposes no setup complications or additional radiation dose compared to absorption-based imaging. Considering the phase-attenuation duality ($\varepsilon = \delta/\beta$, where ε is constant), a simple absorption correction factor is proposed for the modified Bronnikov algorithm in x-ray propagation-based phase-contrast computed tomography (PPCT). Moreover, a practical method for calculating the optimal ε value is proposed, which requires no prior knowledge of the sample. Tests performed on simulation and experimental data successfully distinguished different materials in a quasihomogeneous and weakly absorbing sample from a single SDD-PPCT data point. © 2011 Optical Society of America

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X-ray phase-sensitive computed tomography (CT) can provide substantially enhanced contrast, especially for low-Z samples [1]. The x-ray propagation-based phase-contrast CT (PPCT) method has attracted wide attention thanks to its particularly simple experimental setup—identical to absorption-based CT except for providing that the beam is sufficiently spatially coherent and increasing the sample-to-detector distance (SDD), to let the beam propagate in free space after interaction with the sample [2].

PPCT provides high-contrast qualitative images, i.e., edge enhancement, and has extensive applications in many research fields [3]. Moreover, PPCT radiographies also contain phase information that could be extracted; in fact, phase retrieval is a technique for extracting quantitative phase information from PPCT [2]. Several phase-retrieval algorithms have been proposed, such as the transport of intensity equation (TIE) method [4], the contrast transfer function (CTF) method [2], the mixed approach between the CTF and TIE method [5,6], the Bronnikov algorithm [7], and others [8,9]. However, all these methods require multiple SDD intensity measurements that deliver a higher radiation dose to the samples, which could hinder its biomedical applications. Undoubtedly, phase retrieval utilizing a single SDD-PPCT data point will boost its applications, and make the procedure much easier [10,11], especially for low-Z samples.

The Bronnikov algorithm integrates the phase-retrieval step into a modified CT reconstruction algorithm and provides direct reconstruction of the three-dimensional (3D) refractive index from the PPCT data [7]. Furthermore, Groso *et al.* introduced an absorption correction factor (ACF: α) in the Bronnikov algorithm, naming it the modified Bronnikov algorithm (MBA), and succeeded to apply it for a single SDD-PPCT data point [10]. However, the ACF value in the MBA was determined using a semi-empirical approach, which may be cumbersome and time consuming, because the ACF varies with the samples, and thus it is inconvenient in general applications. Moreover, if it is not sufficiently precise, that will affect the reconstruction results, which will be blurred with a too-small ACF value, while the filter will be eliminated with a too-large value.

In this Letter, based on phase-attenuation duality ($\varepsilon = \delta/\beta$, where ε is constant and $n = 1 - \delta + i\beta$ is the complex refraction index), which is valid for quasihomogeneous and weakly absorbing samples [9], an approach to determine the ACF value simply and accurately is proposed for MBA, which takes the wavelength, SDD, and phase-attenuation duality of PPCT into account. Moreover, a practical method for calculating the optimal ε value directly is proposed, based on the first Born-type approximation phase-retrieval algorithm [8]. Therefore, no prior knowledge of the sample is required for 3D refractive index reconstruction from a single SDD-PPCT data point.

As shown in Fig. 1, when a monochromatic plane x-ray beam illuminates a sample that is quasihomogeneous and weakly absorbing, the intensity distribution $I_{\theta,z}$ at SDD $= z$ and the rotation angle θ is approximated according to the TIE [4]:

$$I_{\theta,z}(x,y) = I_{\theta,0}(x,y)\left[1 - \frac{\lambda z}{2\pi}\nabla^2\phi_\theta(x,y)\right], \tag{1}$$

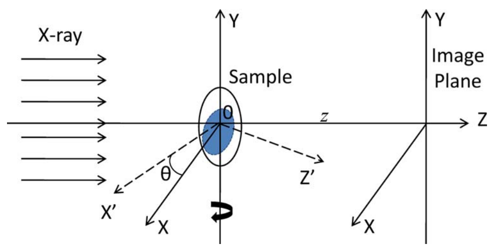

Fig. 1. (Color online) Schematic of the PPCT scanning geometry.

where λ is the wavelength, $I_{\theta,0}(x,y)$ is the intensity in the contact plane, and $\phi_\theta(x,y) = \frac{2\pi}{\lambda}\int \delta_\theta(x,y,z)\mathrm{d}z$ is the sample phase function, which integrates over the object thickness along the beam propagation direction, at rotation angle θ, respectively.

Reformulating Eq. (1) as $\nabla^2\phi_\theta(x,y) = -\frac{2\pi}{\lambda z} g_\theta(x,y)$ with $g_\theta(x,y) = I_{\theta,z}/I_{\theta,0} - 1$, applying the 2D and 3D Radon transform to $g_\theta(x,y)$ and $\delta(x,y,z)$ respectively, the following expression could be deduced, which is the main result of the Bronnikov algorithm [7]:

$$\delta(x,y,z) = \frac{1}{4\pi^2 z}\int_0^\pi [q(x,y) ** g_\theta(x,y)]\mathrm{d}\theta, \qquad (2)$$

where $q(x,y) = \frac{|y|}{x^2+y^2}$ is a filter and $**$ indicate a 2D convolution. Equation (2) can be utilized to reconstruct a 3D refractive index $\delta(x,y,z)$ from two SDD-PPCT data points, i.e., $I_{\theta,0}$ and $I_{\theta,z}$.

Suppose imaging a quasihomogeneous and weakly absorbing sample, i.e., $I_{\theta,0} \approx 1$, according to the convolution theory and taking the effects of nonzero absorption into account, the equation can be evaluated via Fourier space transformation with $g_\theta(x,y) = I_{\theta,z} - 1$ and the following low-pass filter [10]:

$$Q(\xi,\eta) = \frac{|\xi|}{\xi^2+\eta^2+\alpha}, \qquad (3)$$

where (ξ,η) correspond to (x,y) in the Fourier space and α is the AFC, which was introduced by Groso [10]. In the following paragraphs, an approach for determining the α value quickly and accurately is proposed and evaluated.

When a sample is quasihomogeneous, the real and imaginary parts of its complex refraction index are proportional to each other (phase-attenuation duality property) [9], i.e., $\delta(x,y,z) = \varepsilon\beta(x,y,z)$, where ε is a constant. According to the PPCT theory, there are four parameters that affect the result, namely, the wavelength λ, SDD z, effective pixel size of the detector Δ, and complex refraction index of the sample. With the phase-attenuation duality property, the last parameter can be replaced with ε in the phase-retrieval procedure. The dimensional analysis method was used to compute the relationship between α and λ, Δ, z, and ε: (i) assuming $\alpha = a\lambda^b\Delta^c z^d\varepsilon^e$ with unknown values a, b, c, d, and e; (ii) simulating the PPCT data with different λ, Δ, z, ε values; (iii) reconstructing the best PPCT result and obtaining the corresponding α value; (iv) calculating the a, b, c, d, and e values from a series of $\alpha = a\lambda^b\Delta^c z^d\varepsilon^e$ equations. The result we obtain for the AFC is

$$\alpha = \frac{1}{\pi\varepsilon\lambda z}. \qquad (4)$$

Equation (4) takes λ, z, and ε of the PPCT into account, while Δ was considered in the filter $Q(\xi,\eta)$. It should be noted that, Gureyev *et al.* also reached a similar result with theory analysis, which we noticed when checking our result with the literature; however, to the best of our knowledge, they did not test it with simulation or experimental data [12].

In Eq. (4), typically, the ε value is treated as prior knowledge of the sample [11], but this will be a challenge for unknown samples. Here, we propose a practical method to determine it from the experimental data. According to the first Born-type approximation phase-retrieval algorithm, the intensity distribution I_z at SDD $= z$ of PPCT can be approximated by the following equation [8]:

$$\mathcal{F}[(I_z/I_0 - 1)/2](\xi,\eta) = \hat{\gamma}\cos\chi + \hat{\phi}\sin\chi, \qquad (5)$$

where $\chi = \pi\lambda z(\xi^2+\eta^2)$, $\hat{\phi}$, and $\hat{\gamma}$ denote the Fourier transform of phase and absorption function, ϕ and $\gamma = \frac{2\pi}{\lambda}\int \beta(x,y,z)\mathrm{d}z$, which also integrates over the object thickness along the beam propagation direction. In the case of a quasihomogeneous and weakly absorbing sample, i.e., $I_0 \approx 1$, with intensity measurement at two different SDDs (z_1 and z_2), the ε value can be calculated as in the following equation:

$$\varepsilon = \left\langle \frac{\phi}{\gamma} \right\rangle = \left\langle \frac{\mathcal{F}^{-1}\left\{ \left[\cos\chi_1 \mathcal{F}\left(\frac{I_{z_2}-1}{2}\right) - \cos\chi_2 \mathcal{F}\left(\frac{I_{z_1}-1}{2}\right)\right] / \sin(\chi_2-\chi_1) \right\}}{\mathcal{F}^{-1}\left\{ \left[\sin\chi_2 \mathcal{F}\left(\frac{I_{z_1}-1}{2}\right) - \sin\chi_1 \mathcal{F}\left(\frac{I_{z_2}-1}{2}\right)\right] / \sin(\chi_2-\chi_1) \right\}} \right\rangle, \qquad (6)$$

where $\chi_1 = \pi\lambda z_1(\xi^2+\eta^2)$, $\chi_2 = \pi\lambda z_2(\xi^2+\eta^2)$, and $\langle\rangle$ denotes the average value on the sample.

The proposed method was first evaluated via simulation. As shown in Fig. 2(a), the 3D phantom was made up of two spheres intersecting with each other; a PPCT

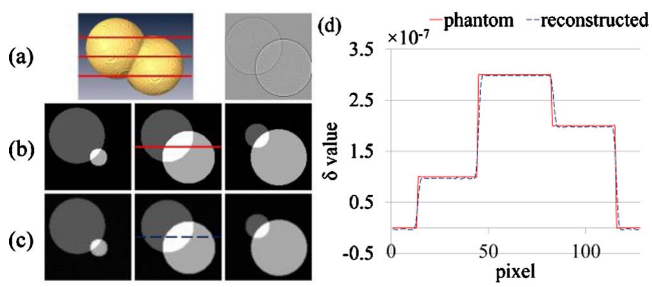

Fig. 2. (Color online) Simulation results: (a) 3D phantom and one PPCT projection. (b) Cross-sectional view of 3D phantom. (c) Corresponding reconstructed results of (b). (d) Profiles of the phantom and the reconstructed result along the line positions in Figs. 2(b) and 2(c), respectively.

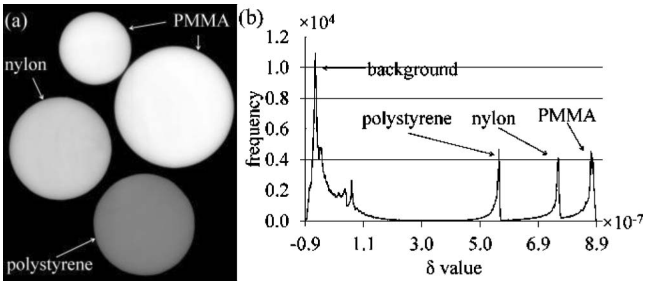

Fig. 3. (Color online) Experimental results: (a) reconstructed result of the wire sample and (b) histogram of Fig. 3(a); the labels indicate the peak for each material.

projection at a given rotation angle is shown on the side. Figure 2(b) shows three phantom slices according to the line positions in Fig. 2(a). Three different values were assigned to the three phantom regions respectively, i.e., the (δ, β) values of the phantom were (0.0, 0.0) (black, background), $(1.0 \times 10^{-7}, 1.0 \times 10^{-10})$, $(2.0 \times 10^{-7}, 2.0 \times 10^{-10})$, $(3.0 \times 10^{-7}, 3.0 \times 10^{-10})$ (white), which means $\varepsilon = 1000$ for the phantom. The PPCT data were generated via the tomography projection theory and the Fresnel diffraction theory with $\lambda = 0.1$ nm, SDD $= 20$ mm, and a pixel size of $2\,\mu$m. At a given rotation angle, an additional projection with SDD $= 50$ mm was simulated, to calculate the ε value via Eq. (6). The result is 1001, very close to the ideal value 1000. Three reconstructed slices [the same position of Fig. 2(b)] are shown in Fig. 2(c). Figure 2(d) depicts the profiles of the phantom and the reconstructed result along the line position in Figs. 2(b) and 2(c), respectively. It can be seen that the reconstructed values of the refractive index match the ideal values well except for some small errors near the edges of the objects, which can be explained by the influence of the interpolation in the backprojection step.

In the second step, the method was evaluated with experimental PPCT data collected at the X-ray Imaging and Biomedical Application Beamline at the Shanghai Synchrotron Radiation Facility. A sample with wires of nylon ($\varnothing = 1.6$ mm), polystyrene ($\varnothing = 1.6$ mm), and poly(methyl methacrylate) (PMMA—$\varnothing = 1$ and 2 mm—GoodFellow, Huntingdon, UK), was investigated at 18 keV with an effective pixel size of $3.7\,\mu$m and SDD $=$ 20 cm. An additional projection with SDD $= 60$ cm was obtained for calculating the ε value via Eq. (6). The result was 2503, and the ideal values of polystyrene, nylon, and PMMA are 2062, 2371, and 2852, respectively at 18 keV [13]. The reconstructed result was shown in Fig. 3(a), while Fig. 3(b) shows the histogram of Fig. 3(a). As both images show, three materials can be well distinguished, although the ε value has not been optimized for every specific material. Moreover, there is a qualitative agreement with the ideal values, which are polystyrene (7.24e − 7) < nylon (8.01e − 07) < PMMA (8.23e − 07).

We have proposed a fast and experimental feasible approach for reconstructing the 3D refractive index for quasihomogeneous and weakly absorbing samples, from a single SDD-PPCT data point. The method was tested with simulation and experimental data. We believe that our method will find applications in a number of different fields, such as biomedical science and material science, because it imposes no additional radiation dose compared to ACT.

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