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Apparent Linear Attenuation Coefficients in Phase Contrast X-Ray Tomography

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Abstract

In the inline phase contrast x-ray tomography the reconstructed apparent linear attenuation coefficient values may be greatly larger than sample's linear attenuation coefficients or even be negative. In this work we present a general formula to quantitatively relate the apparent linear attenuation coefficient values in cone-beam phase contrast tomography to sample's linear attenuation coefficients and refractive indices. This formula overcomes the gross inaccuracy of the existing formula in the literature in analyzing high-resolution phase contrast tomography, and it will be useful for correctly interpreting and quantifying the apparent linear attenuation coefficients in cone-beam x-ray phase contrast tomography.

Keywords

X-ray phase contrast imaging; X-ray tomography

For many applications the x-ray attenuation contrast, such as mass-density differences between different material components, is too small to generate enough image contrast with conventional x-ray tomography. Taking advantage of highly sensitive x-ray phase shifts generated from x-ray coherent scattering, phase contrast x-ray tomography finds broad applications in material science and engineering, biomedical imaging and many other scientific fields [1–3]. In phase contrast x-ray tomography one first makes phase contrast angular projections, in which the refraction and diffraction of phase shifted x-rays form the edge-enhancing interference fringes at interfaces of different material components. From these angular projections 3-D tomograms are then reconstructed using the standard tomography reconstruction methods such as the filtered backprojection methods. The reconstructed phase-sensitive tomograms exhibit enhanced interfaces and layers of different materials and tissues [1–3]. However, these tomograms are not the maps of the linear attenuation coefficients (LACs) of the sample, rather they are the maps of the reconstructed apparent LACs, which may present anomalously large or even negative apparent LAC values at interfaces between different materials and tissues. These “artifacts” may cause faulty interpretation of sample structures, and impede even qualitative characterizations for tissues and materials [1–2, 4–6]. As a result, for example, the apparent LAC values of small

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bronchi were found lower than that of air in phase contrast tomography experiments [2]. In order to correctly interpret and quantify the mixed contrast exhibited in phase contrast tomography, it is necessary to find out quantitative relations between the apparent LAC, on the one hand, and the actual LAC and refractive index, on the other. The previous studies found that the apparent LAC $\mu_{\text{apparent}}(\vec{r}_o)$ in x-ray phase contrast tomography is given by [7–9]:

$$\mu_{\text{apparent}}(\vec{r}_o) = \mu(\vec{r}_o) - \frac{R_2}{M} \cdot \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \right) \Delta_{\text{refr}}(\vec{r}_o). \quad (1)$$

In this equation the first additive term $\mu(\vec{r}_o)$ denotes the sample's actual LAC value at position $\vec{r}_o$, and the second additive term is proportional to the three-dimensional Laplacian of the sample's refractive index decrement $\Delta_{\text{refr}}(\vec{r}_o)$ [7–9]. In Eq. (1) R_2 denotes the sample-detector distance and M the magnification factor employed in angular projections. In the literature this second term is used to explain the edge enhancement and the anomalous values of large apparent LAC [7–9].

However, in high-resolution phase contrast tomography with micrometer-scale resolutions the applicability of Eq. (1) is called into question. Researchers recently found that Eq. (1) is invalid in some synchrotron radiation microtomography experiments [10]. In fact, in the derivation of Eq. (1) the phase-sensitive projections were modeled based on the so-called Transport of Intensity Equation (TIE) [7–9]. The TIE describes how the phase-shifted x-rays refract and diffract to form interference fringes at boundaries of material components [11–12]. However, we noted that TIE can only describe the moderate-resolution phase-sensitive projections with $\pi\lambda R_2/(4M\sigma^2) \ll 1$, where σ denotes the finest size resolved. In cases of high-resolution projections with micrometer-scale resolutions, the fine size resolved could be so small such that $\pi\lambda R_2/4M\sigma^2 \sim 1$ or larger, then TIE becomes inapplicable and Eq. (1) cannot quantify the apparent LAC values observed in high-resolution phase contrast tomography.

To overcome the limitations of Eq. (1), we derived a novel and general formula of apparent LAC values in phase contrast x-ray tomography. Instead of using the TIE, in the derivation we employed the general phase-sensitive projection formula that is applicable for high-resolution projections as well [13–14]. We then applied the standard Feldkamp-Davis-Kress (FDK) cone-beam reconstruction algorithm to the ray-sums of phase-sensitive angular projections [15]. We found that the apparent LAC value $\mu_{\text{apparent}}(\vec{r}_o)$ is given by

$$\mu_{\text{apparent}}(\vec{r}_o) = \cos\left(\frac{\lambda R_2}{4\pi M} \nabla_{3D}^2\right) \mu(\vec{r}_o) - \frac{4\pi}{\lambda} \sin\left(\frac{\lambda R_2}{4\pi M} \nabla_{3D}^2\right) \Delta_{\text{refr}}(\vec{r}_o), \quad (2)$$

where the three-dimensional Laplacian operator $\nabla_{3D}^2 \equiv (\partial^2/\partial x_1^2 + \partial^2/\partial x_2^2 + \partial^2/\partial x_3^2)$. The operators $\sin((\lambda R_2/4\pi M) \nabla_{3D}^2)$ and $\cos((\lambda R_2/4\pi M) \nabla_{3D}^2)$ in above equation are the pseudo-differential operators. The action of a pseudo-differential operator such as $\sin(c \nabla_{3D}^2)$ on a function $g(\vec{r}_o)$ is defined as

$$\sin(c \nabla_{3D}^2) g(\vec{r}_o) \equiv \iint \exp(i2\pi(\vec{r} - \vec{r}_o) \cdot \vec{f}) \cdot \sin(-4\pi^2 c \vec{f}^2) g(\vec{r}) d^3\vec{r} d^3\vec{f}. \quad \text{Note that Eq. (2) is indeed a generalization of Eq. (1). For experiments with moderate-resolutions or short sample-detector distances such that } \pi\lambda R_2/4M\sigma^2 \ll 1, \text{ we then have } \cos((\lambda R_2/4\pi M) \nabla_{3D}^2) \approx 1$$

and $\sin((\lambda R_2/4\pi M)\nabla_{3D}^2) \approx (\lambda R_2/4\pi M)\nabla_{3D}^2$. Thereby the first term on the RHS of Eq. (2) reduces to the actual LAC, the second term to a scaled Laplacian of $\Delta_{refr}(\vec{r}_o)$ and Eq. (2) recovers Eq. (1), as is expected.

In order to validate Eq. (2), we performed numerical simulations. In the simulations the x-ray source was a point source of 60 keV x-rays. The LACs and refractive indices of the numerical phantom were constructed as the sums of the LACs and refractive indices of six spheres of light elements with different radii and center positions. For each sphere the mass densities were designed to decrease radially and diminish rapidly at the sphere's boundary

for generating phase contrast. Specifically we set $\mu(\vec{r}_o) = 0.215 \times \sum_{n=1}^6 f_n(\vec{r}_o) (1/\text{cm})$ and

$\Delta_{refr}(\vec{r}_o) = (7.548 \times 10^{-8}) \times \sum_{n=1}^6 f_n(\vec{r}_o)$, where $f_n(\vec{r}_o) = \sqrt{R_n^2 - (\vec{r}_o - \vec{r}_n)^2} / 4R_n$ if $|\vec{r}_o - \vec{r}_n| \leq R_n$ and $f_n(\vec{r}_o) = 0$ otherwise. Here $\vec{r}_n$ and R_n ($n = 1, 2, \dots, 6$) denote the center position and radius of the respective sphere. In this way the LACs and refractive indices change continuously without any steps but vary rapidly at the sphere boundaries. Hence strong phase contrast would manifest around the boundaries of the spheres. The detector has 512×512 pixels with a sampling pitch of $2\mu\text{m}$. In the simulated scan the source traced a circle orbit, and the source and detector rotated together over an angular range of 360° in 0.5° steps. In order to simulate x-ray Fresnel diffractions involved in the angular projections, one needs to compute x-ray attenuation values and phase shifts of the exit rays in each of the projections. In general one needs to use the multislice propagation method to account for x-ray Fresnel diffractions inside the sample [16]. However, the settings described above satisfy the so-called thin object condition $T < p^2/2\lambda_o$, where T denotes the sample's thickness, p is the resolution and λ_o the wavelength of 60 keV x-ray [16]. This condition allows us to compute the x-ray attenuation values and phase shifts of the exit x-rays as the ray integrals of the sample's LACs and refractive index decrements. In this simulation a ray-tracing algorithm was used to compute the ray integrals such as $\int \mu dl$ and $\int \Delta_{refr} dl$ in each of the angular projections. The exit x-ray attenuation and phase shift were determined as $A^2 = \exp(-\int \mu dl)$ and $\phi = -(2\pi/\lambda) \int \Delta_{refr} dl$, respectively [11–14]. Using the exit x-ray attenuation and phase shift from a given projection, we then simulated the free-space Fresnel diffractions of the exit x-rays propagating from the sample to the detector with a setting of $R_2 = 1\text{m}$ and $M = 2$ [16]. The Fresnel diffraction intensities in all the angular projections were log-transformed to calculate the ray-sums needed for tomographic image reconstruction.

We applied the standard FDK algorithm for image reconstruction [15]. Fig. 1 shows a reconstructed slice of apparent LAC values in gray scale. This slice shows the edge-enhancing dark-bright fringes caused by phase contrast at the interfaces between the spheres. Fig. 2(a) shows the profile of the apparent LAC values along the vertical central line of Fig. 1. The ordinate denotes apparent LAC value in $(1/\text{cm})$ along the vertical line, while the abscissa denotes pixel location along the line. For the sake of comparison Fig. 2(b) and Fig. 2(c) show the profiles of the apparent LAC values along the vertical line, which were computed by using Eq. (1) and Eq. (2) respectively. Note that the ordinate scale in Fig. 2(b) is three times larger than that of Figs. 2(a) and 2(c). To facilitate the comparisons of the three profiles, we measured the fringe's peak-to-peak differences (the changes between peak and trough) at eight fringe sets for each of the three profiles shown in Figs. 2(a)–(c). Table 1 lists the measured fringe peak-to-peak differences of apparent LACs in Fig. 2(a), which is obtained from Fig. 1, the phantom's phase contrast tomogram simulated by using the Fresnel diffraction and FDK-reconstruction. Compared to these eight peak-to-peak differences in Fig. 2(a), the table lists as well the errors of the calculated peak-peak differences based on

Eq. (1) (Fig. 2(b)) and Eq. (2) (Fig. 2(c)) respectively. From these comparisons, it is clear that the apparent LAC values calculated from Eq. (1) are grossly inaccurate with the errors amounting to several hundred percent, while the apparent LAC values calculated by means of Eq. (2) achieve reasonable quantitative accuracies as is shown in Table 1. In addition, the profile Fig. 2(c) shows two small bumps at the center of the profile. We found that these variations of apparent LACs are artifacts caused by omitting the small nonlinear terms in phase shifts in the derivation of Eq. (2). The omission of these nonlinear terms mainly affects the accuracies in computing the side-lobes of phase contrast fringes, thereby causes these two small bumps, which are associated with the distorted fringe side-lobes near the right boundary of the left off-center sphere in the phantom (Fig. 1).

In summary, we present a general formula (Eq. (2)) to quantitatively relate the apparent LAC values in cone-beam phase contrast tomography to sample's LAC and refractive index values. This formula overcomes the gross inaccuracy of the existing formula in the literature in analyzing high-resolution phase contrast tomography. We believe that this general formula will be useful for designing phase contrast tomography experiments, and for correctly interpreting and quantifying the apparent LAC values in cone-beam x-ray phase contrast tomography. For example, Eq. (2) can be used for computing the edge-enhancement profiles for analyzing presampling modulation transfer functions in synchrotron radiation microtomography [10].

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Figure 1. Reconstructed apparent LAC map of a phantom slice from the phase-sensitive cone-beam tomography with mixed contrast.

Figure 2.

Profiles of the apparent LACs along the vertical line passing the center of the central sphere.

(a) Profile measured from Fig. 1. (b) Profile calculated based on Eq. (1). (c) Profile

calculated based on the general formula Eq. (2).

Table 1

A comparison of the fringe peak-peak differences in Figs. 2(a)–(c)

	Fringe set 1	Fringe set 2	Fringe set 3	Fringe set 4	Fringe set 5	Fringe set 6	Fringe set 7	Fringe set 8
Peak-peak difference of apparent LACs in Fig. 2(a) (1/cm)	4.648	4.979	6.098	8.860	8.860	6.098	4.979	4.648
Error of calculated peak-peak difference based on Eq. (1) (Fig. 2(b))	429%	346%	199%	136%	136%	199%	346%	429%
Error of calculated peak-peak difference based on Eq. (2) (Fig. 2(c))	15.0%	17.5%	13.0%	6.9%	6.9%	13.0%	17.5%	15.0%