One-Step Method for Material Quantitation Using In-Line Tomography With Single Scanning

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Abstract—Objective: Quantitative technique based on In-line phase-contrast computed tomography with single scanning attracts more attention in application due to the flexibility of the implementation. However, the quantitative results usually suffer from artifacts and noise since the phase retrieval and reconstruction are independent (“two-step”) without feedback from the original data. The work aims to investigate a method for material quantitation to improve the image quality of In-line tomography within single scanning. Method: An iterative method based Fresnel diffraction imaging model is developed in this work, which directly reconstructs the refractive index decrement $\delta$ and imaginary $\beta$ of the object from observed data (“one-step”). Moreover, high-quality material decomposition results are obtained by using a linear approximation in the iterative process. Results: Compared with the existing methods, Our method shows a higher peak signal-to-noise ratio and structural similarity in numerical experimental results. Additionally, the quantitation accuracy of the proposed method is greater than 97.2% by calculating the equivalent atomic number of the decomposed basic material in the real experiment. Conclusion: We demonstrate that this one-step method greatly reduces noise and improves quantitative reconstruction and decomposition results. Significance: This algorithm has the potential for quantitative imaging research using In-line tomography in future biomedical applications.

Index Terms—Computed tomography, material quantitation, linear approximation, single scanning, phase-contrast, one-step method.

I. INTRODUCTION

X-ray computed tomography (CT) technology is widely used in medicine and industry. Conventional polychromatic X-ray CT imaging is based on the difference in radiation absorption between substances or tissues. Since this imaging modality relies on the X-ray spectrum, it is insufficient for quantitative imaging of materials, especially low-Z substances (low-atomic-number material, such as human soft tissues). Therefore, new imaging mechanisms and techniques need to be introduced to meet the needs of CT material quantitative imaging. During the last decades, dual-energy CT and phase-contrast imaging have been developing rapidly and made significant progress in material quantitation [1]–[6]. There are some methods for material decomposition that combine spectral and phase-contrast information. Mechlem et al. confirmed that spectral grating-based phase-contrast imaging could strongly reduce the noise level of the image [7]. Compared with conventional CT, they have some additional requirements. In dual-energy CT, projection data need to be acquired twice with different $k$Vp (kilovoltage peak) by using an energy-integration detector or only once by using a photon-counting detector (PCD) [8], [9]. Gratings play a crucial role in material quantitation in the grating-based imaging [10]–[13].

In the X-ray energy range of 5–200 keV, the differences in X-ray phase shifts in low-z materials are about three orders of magnitude larger than their absorption changes [14], [15], which means the additional sensitivity is available. Many techniques can measure the phase-shifting properties of the sample, in addition to grating-based imaging [16], [17], there are crystal interferometry [18], [19], analyzer-based phase-contrast [20], [21] and In-line phase-contrast imaging, also known as propagation-based phase-contrast imaging (PPCI) [22]–[24]. Unlike other techniques, PPCI does not require other optical components to facilitate the implementation.

Numerous propagation-based phase retrieval algorithms need to measure X-ray intensity at two or more object-to-detector distances (ODD), which will increase the radiation dose received by the object, data collection time and processing difficulty [25]–[27]. Meanwhile, the multi-energy propagation-based phase-contrast methods have the same disadvantages due to the multi-scans on a single ODD [4], [28]. Many studies focus on developing phase retrieval algorithms based on single scanning to overcome the above problems. As we know, the phase retrieval problem of PPCI becomes an ill-posed inverse problem in single scanning since it is a challenge to retrieve the
phase and absorption of the sample simultaneously from single original data. Therefore, prior knowledge is required [29]–[31]. One of the most widely used prior knowledge is homogeneity assumption $\delta = a \ast \beta$, which assumes that the sample is composed of a single material. Generally, many specimens often consist of two or more materials in actual application. There are quantitative phase retrieval algorithms for multi-material samples that incorporate an improved assumption $\delta_1 = \delta_0 + \frac{\lambda^2}{2}\mu_1$ [32]. Beltran et al. proposed a method that retrieve the difference $(\mu_2 - \mu_1)T_2$ in projected attenuation between two materials and the total projected thickness of the object in each direction need to be known [33]. The total attenuation retrieval and correcting interface for all materials by using the improved assumption was proposed by Ulherr et al. [34].

PPCI and CT can work together to obtain the $\delta$ tomography of samples [35]–[41]. But it is usually implemented in two steps: firstly, the phase shifting is retrieved from the X-ray intensity; secondly, the object is reconstructed by a conventional algorithm such as Filter Back Projection (FBP) or Algebraical Reconstruction Technique (ART) [42]. However, the reconstructed images usually suffer from artifacts and noise since the projected phase retrieval and reconstruction are independent without feedback from the observed data. It is widely acknowledged that one-step concepts have many advantages and are still being studied in the X-ray imaging field. In multi-energy CT (incl. photon-counting CT), several groups have demonstrated that an iterative one-step reconstruction can improve quantitative results [43]–[45]. Previous works in grating-based phase-contrast reconstruction show that it is possible to reconstruct without stepping when using a one-step algorithm [46]–[49]. Notably, these algorithms are related to different imaging physics and mathematical models. Multi-energy CT is based on the imaging principle that the energy attenuation behavior of the materials varies with different X-ray spectrums. However, this principle is challenged in the real application with low-Z compounds, which have weak absorption. Grating-based imaging is based on the grating self-imaging effect in optics, which also means that additional optics devices are required for imaging. The experimental operation is complicated and the grating will reduce the utilization rate of X-ray.

Hence, the authors believe that it is potential to use the one-step concept for quantitative imaging of low-Z samples without additional optical components in PPCI. In this work, we investigate a one-step method based on single scanning, which can simultaneously reconstruct the images of the absorption factor $\beta$ and the refractive index decrement $\delta$ from original data for propagation-based phase-contrast tomodgraphy (AR-PPCT). Meanwhile, aiming at the high-precision quantitative reconstruction of multi-material, we combine this iterative method with the improved approximation for accurate dual-material decomposition.

II. THEORY AND METHODS

A. Imaging Theory of PPCI

The interaction between X-rays with matter can be described by the following complex refractive index:

$$n = 1 - \delta + i\beta.$$  \hspace{1cm} (1)

Here $\delta$ is the phase shifting factor, $\beta$ the absorption factor, and $\beta = \frac{\beta_2 - \beta_1}{2\mu_2}$ the wave number. The wavelength, $\mu$ the linear attenuation coefficient. In terms of value, $\delta$ is much larger than $\beta$. When an X-ray plane wave $A^\text{in}$ pass through the object, the wave function of the emergent beam reads

$$A(x, y) = A^\text{in} \exp\left(-\frac{M(x, y)}{2} + i\Phi(x, y)\right),$$  \hspace{1cm} (2)

where $M(x, y)$ and $\Phi(x, y)$ are the X-ray absorption and phase shift, respectively.

$$M(x, y) = \frac{4\pi}{\lambda} \int_{l} \beta(x, y, z)dz, \hspace{1cm} (3)$$

$$\Phi(x, y) = -\frac{2\pi}{\lambda} \int_{l} \delta(x, y, z)dz, \hspace{1cm} (4)$$

Here $l$ is the integration path. After penetrating the object, the intensity of X-ray decays to

$$I_{\text{out}}(x, y) = |A(x, y)|^2 = I^\text{in} \exp(-M(x, y)), \hspace{1cm} (5)$$

here $I^\text{in} = |A^\text{in}|^2$ is the intensity of incoming X-rays.

In the case of paraxial approximation, according to the Fresnel diffraction theory, the plane X-ray intensity distribution at the distance $z$ from the sample can be written as [38]:

$$I_z(x, y) = |h_z \otimes A(x, y)|^2, \hspace{1cm} (6)$$

where $\otimes$ represents convolution, $h_z$ is the Fresnel propagator:

$$h_z = \frac{\exp(ikz)}{ikz} \exp\left(\frac{\pi}{\lambda z}(x^2 + y^2)\right), \hspace{1cm} (7)$$

Here $k = \frac{2\pi}{\lambda}$ is the wave number.

The mathematical problem of PPCT is to reconstruct the $\delta$ and $\beta$ of the measured sample from a serial of intensity $I_z$ with different paths $l$.

B. The Linear Relationship Approximation

By single scanning in propagation-based phase-contrast imaging, the phase retrieval problem becomes an ill-posed inverse problem since there is only one set of intensity data and two unknown variables ($\delta$ and $\beta$). Establishing a certain hypothetical relationship between $\delta$ and $\beta$ is necessary. One of the most widely used assumptions is a proportional relationship: $\delta = a \ast \beta$, which means that the object consists of only a single material. However, most objects often consist of more than one material in the application. How to achieve the high-precision value of $\delta$ and $\beta$ is of great significance for PPCI with single scanning.

Firstly, we suppose whether we can define a higher-order approximation to the $\delta$ and $\beta$ of the multi-base materials. The approximation is expressed as follows:

$$\delta = a_N\beta^N + a_{N-1}\beta^{N-1} + a_{N-2}\beta^{N-2} + \ldots + a_1\beta + a_0, \hspace{1cm} (8)$$

the above formula is an expression of an equation of degree N in one variable $\beta$.

Dual-material decomposition, which allows quantitative material images and beam-hardening artifact reduction, has many
Two different material combinations can achieve the corresponding decomposition with this linear relationship. Therefore, after preselecting dual-material, we pay attention to material decomposition and quantitation for multi-material samples.

C. Reconstruction Algorithm

According to the Born approximation, the X-ray intensity $I_z$ in the image plane ($z$ represents the distance from the sample to the image plane) satisfies the following mathematical relationship [50]:

$$
\mathcal{F} \left[ \frac{I_z}{I_0} - 1 \right] = \cos(z \rho^2) \Re \psi_0 + \sin(z \rho^2) \Im \psi_0,
$$

(12)

where $\Re \psi_0 = \mathcal{F}[-k \int \delta dl]$, $\Im \psi_0 = \mathcal{F}[-k \int \delta dl]$. $\rho^2 = \pi \lambda (\zeta^2 + \eta^2)$, $(\zeta, \eta)$ are the frequency domain coordinates of $(x, y)$. $\mathcal{F}$ is the Fourier transform.

Let $\beta = (\beta_1, \beta_2, \ldots, \beta_j)^T$ and $\delta = (\delta_1, \delta_2, \ldots, \delta_j)^T$ denote the discretized images of $\beta(x, y)$ and $\delta(x, y)$, where $\beta_i$ and $\delta_i$ are the sampled values of $\beta(x, y)$ and $\delta(x, y)$ at the $i$th pixel. $J$ is the total pixel number, and $\tau$ is the vector transpose operation. $R^\varphi = (r_{\varphi j})_{U \times J}$ is the projection matrix at angle $\varphi$, where $(r_{\varphi j})$ represents the contribution of $\delta_j$ and $\beta_j$ to the projection along the $j$th x-ray path at projection angle $\varphi$. $I_z^* = U$ dimensional column vector, $U$ is the number of detector cell. Firstly, we obtain the residual X-ray intensity by subtracting the measured intensity and the simulated intensity. the intensity residual of the $m$-th iteration at projection angle $\varphi$ is:

$$
\text{Re} \psi^m(m) - \text{Re} \psi^m(m) = \mathcal{F} \left( \frac{\text{Re} \psi^m(m)}{2} \right)
$$

(13)

here $M^{\varphi} = 2k \int \beta^\varphi dl$ and $\Phi^\varphi = -k \int \delta^\varphi dl$.

Utilizing the linear relation Eq. (9), we can attain $\Im \psi_0 = a \text{Re} \psi_0 + \mathcal{F}[-k \int \delta dl]$ and the absorption residual of the $m$-th iteration at projection angle $\varphi$ is:

$$
\text{Re}/\varphi - \text{Re} \psi^m(m) = \frac{\mathcal{F} \left( \text{Re} \psi^m(m) / 2 \right)}{\cos(z \rho^2) + \sin(z \rho^2) \ast a},
$$

(14)

where $\mathcal{F}$ is 1D Fourier transform, and $\text{Re} = \mathcal{F}^{-1}(\text{Re} \psi^\varphi - \text{Re} \psi^m(m))$ is $U$ dimensional column vector, $\mathcal{F}^{-1}$ is 1D Inverse Fourier transform. Then combining the Simultaneous Algebraical Reconstruction Technique (SART) [51], we can directly reconstruct $\delta$ and $\beta$ of the sample for $m+1$ iterations, the scheme is as follows:

$$
\left\{ \begin{array}{l}
\beta^{m+1}_j = \beta_j^m + \gamma \left( \frac{\mathcal{F}}{R^\varphi_{v,j}} \sum_{u=1}^{U} \frac{r_{\varphi u,j}}{u_{v,j}^2} \text{Re} u \right), \\
\delta^{m+1}_j = \beta^{m+1}_j \ast a + b
\end{array} \right.
$$

(15)

where $R^\varphi_{u,j} = \sum_{j=1}^{J} r_{\varphi u,j}$ with $u = 1, 2, \ldots, U$, and $R^\varphi = \sum_{u=1}^{U} r_{\varphi u,j}$ with $j = 1, 2, \ldots, J$. $\gamma$ the relaxation factor, which can be obtained by simulating the real reconstruction environment experimentally, and then selecting the relaxation factor with the best reconstruction effect and applying it to the real experiment. The above formulas represent the reconstruction of $\delta$ and $\beta$ based on the projection angle $\varphi$, and we need to
Algorithm 1: The AR-PPCT Algorithm.

1: Initialization \( \beta^0 = 0, \delta^0 = 0, m = 0; \)
2: Use Eq. (6)-(7) to calculate the intensity \( I^z(m) \), and gain the residual intensity \( \Re e(z(m) \).
3: Iteratively update \( \beta^{m+1} \) and \( \delta^{m+1} \) according to Eq. (15);
4: Use Eq. (16) to remove the non-zero value of air in the image, and then material decomposition by Eq. (11);
5: Set \( m = m + 1 \) and turn to step 2 until the stop condition is met;
6: Return \( \beta^m \) and \( \delta^m \).

reconstruct the tomography from multiple different projection angles.

The shrink function is a mask to remove the non-zero value of the air in the reconstructed image:

\[
\text{shrink}(y, x) = \begin{cases} 
  y = 0 & (b - x < y < b + x) \\
  y = y & \text{else}
\end{cases},
\]

(16)

here \( y \) is the reconstructed image and \( x \) is the parameter. When \( y \) is the \( \delta \) image, the value of \( x \) is less than 100 times that of the constant term \( b \) in Eq. (9).

Finally, we summarize the implementation steps of the algorithm:

III. EXPERIMENTS

In this section, the proposed algorithm is evaluated by numerical simulations and real experiments. As a comparison, we have also tested the Born approximation method with single ODD [52], Linear method [34] and Material Decomposition using Spectral propagation-based phase imaging (MD-SPBI) method [28] in experiments. In this paper, three comparison algorithms use SART algorithms for reconstruction after phase and absorption/decomposed materials projection is retrieved. A commonly defined stopping criterion in mathematics is

\[
\frac{\| \Re e - \Re e^m \|}{\| \Re e \|} \rightarrow 0
\]

Here we choose to set the maximum iteration number to 200 as the stopping criterion.

According to the original reference, MD-SPBI, which uses a set of basis functions defined by the specific materials, can obtain the projection image of base material decomposition. The Born approximation with a single ODD and Linear method are phase retrieval algorithms without material decomposition. The \( \delta = a\beta + b \) is used for Born approximation with a single ODD, and the \( \delta \) is fitted by the least square method. The parameter \( a \) in \( \delta = a\beta + b \) is fitted by the least square method. The phase projection can be obtained by this proportional relationship after calculating the absorption projection in Born approximation single-distance method. Meanwhile, the \( \delta \) image is obtained using this linear relationship again after removing the artifacts of \( \beta \) image in the linear method. After getting \( \beta \) and \( \delta \) images, we use Eq. (11) to obtain the decomposition results of the methods. Furthermore, since MD-SPBI is a multi-energy method, the second energy should be chosen in experiments. We refer to the energy value range in the thesis of MD-SPBI method for the following two reasons: 1) An energy range determined according to imaging requirements and actual conditions; 2) The specific value takes into account the energy value of the comparison methods.

A. Numerical Simulation

As shown in Fig. 2, a FORBILD head phantom was utilized in the numerical experiment [53]. The experimental parameters are displayed in Table I. In the simulation, a parallel-beam setting was used for acquiring 360 projections equally spaced in 180 degrees. The size of sample was 2.45 mm \(* 1.95 \) mm. We simulated both noise-free data and Poisson noise data corresponding to emission flux of \( 10^6 \) photons per measurement. The water and bone were selected as the basic materials for quantitative imaging. The values of \( \delta \) and \( \beta \) were from the X-ray database provided by http://henke.lbl.gov/optical_constants/getdb2.html. The size of the reconstructed image was 512 \(* 512 \). We chose the second energy as 25 keV in MD-SPBI.

Figs. 3–5 show the retrieved projections and the profiles of the projections in noise-free and noisy cases, respectively. It is noted that absorption and phase, water, and bone projection maps are obtained by Radon transformation in AR-PPCT. The tomographies of \( \beta \) and \( \delta \) in noise-free are shown in Fig. 6. The decomposed results of noise-free and noisy cases are shown in Figs. 7 and 8, respectively. In each case, the results of Born approximation with a single ODD, Linear method, MD-SPBI method, and our method are performed. The Peak Signal to Noise Ratio (PSNR) and Structural Similarity (SSIM) of water-based and bone-based materials for these methods in two cases are shown in Tables II and III.

From the results in Figs. 3–5, it can be seen that the absorption and phase projection results of Born approximation with single ODD are far from the ideal results due to the unsatisfactory assumption \( \delta = a\beta \). The MD-SPBI method can better separate water and bone materials by using two sets of different X-ray intensity data, which makes the phase retrieval problem in single scanning PPCI well-posed. Moreover, by comparing
TABLE II
PSNR AND SSIM COMPARISON OF RECONSTRUCTED WATER BASED IMAGE RESULTS

|                | Noise free | Noisey      |
|----------------|------------|-------------|
|                | Born approximation | Linear method | MD-SPBI | AR-PPCT | Born approximation | Linear method | MD-SPBI | AR-PPCT |
| PSNR           | 4.55       | 14.01       | 14.11    | 15.50   | 4.55               | 14.01       | 6.10    | 15.50   |
| SSIM           | 0.002      | 0.91        | 0.92     | 0.94    | 0.002              | 0.91        | 0.65    | 0.94    |

TABLE III
PSNR AND SSIM COMPARISON OF RECONSTRUCTED BONE BASED IMAGE RESULTS

|                | Noise free | Noisey      |
|----------------|------------|-------------|
|                | Born approximation | Linear method | MD-SPBI | AR-PPCT | Born approximation | Linear method | MD-SPBI | AR-PPCT |
| PSNR           | 16.11      | 18.64       | 23.48    | 22.17   | 16.11              | 18.64       | 22.01   | 22.17   |
| SSIM           | 0.70       | 0.86        | 0.97     | 0.95    | 0.70               | 0.86        | 0.95    | 0.95    |

the decomposition results of water materials, it is apparent that the anti-noise ability of the MD-SPBI method is weaker than that of AR-PPCT. From Fig. 5(b), (c), we also find that the profiles of phase and water projections in AR-PPCT and phase projections in Linear method are slightly higher than that of phantom since the non-zero value of the air in δ image isn’t removed completely.

In the noise-free case, the results are depicted in Fig. 6. Compared with the value of phantom, an obvious finding is that the β images of AR-PPCT and Linear method are superior to that of the Born approximation method with single ODD. The δ results of AR-PPCT and Linear method are better than the Born approximation with single ODD because the former two methods use the improved assumption \( \delta = a\beta + b \). Material decomposition can be performed after obtaining δ and β by Eq. (11). The decomposed results are shown in Fig. 7. It is clear that Linear method, MD-SPBI, and AR-PPCT can decompose water-based and bone-based materials, including zoom area. In the noisy case, we are looking at Fig. 8, AR-PPCT, Linear method, and Born approximation with single ODD have certain anti-noise performance. In contrast, MD-SPBI is more sensitive to noise than other methods. Moreover, In Fig. 9(a), (b), the profiles of decomposed results from orange lines in the noisy case show that AR-PPCT, compared with the other methods, has a superior image quality in material quantitation.

The results of PSNR and SSIM, as shown in Tables II and III, indicate that the AR-PPCT has more advantages in material decomposition. The curves of the Root Mean Square Error (RMSE) and SSIM in Fig. 9(c), (d) show the error tends to stabilize as the number of iterations increases. Therefore, the convergence of AR-PPCT is also proved in numerical.

B. Real Experiment 1

The tests were carried out at the beamline 4W1A at the Beijing Synchrotron Radiation Facility (BSRF). As shown in
Fig. 5. Profiles of projections in noise-free case and noisy case. (a) and (b) are the profile lines of absorption and phase projections in noise-free case. (c) and (d) are the profile lines of water-based and bone-based material in noise-free case. (a'), (b'), (c') and (d') are the profile lines of absorption, phase, basic materials in noisy case, respectively.

Table IV

THE EXPERIMENTAL PARAMETERS IN THE BEIJING SYNCHROTRON RADIATION FACILITY (4W1A)

| Parameter               | Value    |
|-------------------------|----------|
| Energy                  | 15 keV   |
| ODD                     | 43 cm    |
| Pixel Array Detector    | 2048×2048|
| Detector Unit Size      | 6.5 mm   |
| Single Exposure Time    | 30 ms    |
| Samples & Size          | PMMA: 4 mm; LDPE: 2 mm |

Fig. 10(a), (b), the experimental samples include PMMA and LDPE. The experimental parameters are displayed in Table IV. The diameters of PMMA and LDPE were 4 mm and 2 mm. The data of 720 angles were collected at equal intervals within 180 degrees. The reconstructed image size was 512×512. We chose the second energy as 10 keV in MD-SPBI.

We extract one layer of the 3D phantom for the reconstruction of δ and β images, and those retrieved projections are shown in

Fig. 11. The reconstructed tomographies and material decomposition are shown in Figs. 12 and 13, respectively.

Fig. 12(g), (h) show the profiles of the β and δ tomographies from orange lines in Fig. 12. The material decomposition results of the four methods are shown in Fig. 13. In Fig. 14, these are the profiles of the PMMA and LDPE images from the orange line in Fig. 13. Strong evidence of AR-PPCT’s ability to decompose substances was found by comparing the profile results. There is a relationship between μ and δ, electron density ρ_e is the intermediate variable [54]:

\[
\begin{align*}
\mu(E,x,y) &= C_p E^C \rho_e(x,y) Z(x,y)^{C_z} + C_{KN}(E) \rho_e(x,y), \\
\delta(E,x,y) &= C_{PC}(E) \rho_e(x,y)
\end{align*}
\] (17)

here \( C_p, C_E \) and \( C_z \) are the parameters to be determined. \( C_{PC}(E) = \frac{r_0 h^2 c^2}{2\pi E^2} \), \( r_0 \) the classical radius of the electron, \( h \) the Planck constant, \( c \) the speed of light, and the Klein-Nishina cross section as follow,

\[
C_{KN}(E) = 2\pi r_0^2 \left( \frac{1 + a}{a^2} \right) \left( \frac{2(1 + a)}{1 + 2a} - \frac{\ln(1 + 2a)}{a} \right) + \frac{\ln(1 + 2a)}{2a} - \frac{1 + 3a}{(1 + 2a)^2},
\] (18)

with \( a = E/511 \) keV the relative mass energy to electron. The theoretical equivalent atomic number \( Z \) for a compound was
calculated by the following equation [55]:

$$Z = \left( \sum_j w_j Z_j^{2.94} \right)^{1/2.94},$$  \hspace{1cm} (19)

here $w_j$ is the fraction of the total number of electrons associated with each element, and $Z_j$ the atomic number of element. The $\beta$ and $\delta$ coefficient of the two materials (PMMA, LDPE) are used in Eq. (17) with 10 keV and 15 keV to fit the coefficient in the $\mu$ formula. After fitting, the coefficients are $C_p = 2.1086e^{-15}$ cm², $C_E = 3.337$ and $C_Z = 3.673$. As shown in Table V, compared with other methods, the fitted results of AR-PPCT are very close to the theoretical values. The relative error is measured by the following formula:

$$\text{err} = \frac{|Z_T - Z|}{Z_T} \times 100\%,$$ \hspace{1cm} (20)

The relative errors of PMMA and LDPE in AR-PPCT are 0.9%~2.7% and 2.0%~2.8%, respectively. In other words, the accuracy of basic materials is greater than 97.2% in AR-PPCT.

C. Real Experiment 2

The experiment was performed on the beamline BL13 W at the Shanghai Synchrotron Radiation Facility (SSRF). The experimental parameters are displayed in Table VI. The data of 540 angles were collected at equal intervals within 180 degrees. The reconstructed image size was 512 * 512. The second energy was 12 keV in MD-SPBI.

As shown in Fig. 10(c), the phantom consists of four components, LDPE, PMMA, PTFE, and water. The PMMA, LDPE, and PTFE cylinders with diameters of 5.6 mm, 4.0 mm, and 2.0 mm, respectively, were placed in a polyethylene plastic tube.

### Table V

| Material | ZT (Theoretical) | Linear Method | MD-SPBI | AR-PPCT |
|----------|-----------------|---------------|---------|---------|
| PMMA | 6.467 | 6.287±0.07 | 6.325±0.35 | 6.523±0.12 |
| LDPE | 5.444 | 5.100±0.03 | 5.434±0.14 | 5.424±0.13 |

$Z_T$ is the theoretical value by (19).

### Table VI

| Parameter | Value |
|-----------|-------|
| Energy | 20 keV |
| ODD | 35 cm |
| Pixel Array Detector | 2048*800 |
| Detector Unit Size | 6.5 um |
| Single Exposure Time | 3.5 ms |
| Samples & Size | PMMA: 5.6 mm; LDPE: 4.0 mm; PTFE: 2.0 mm |
Fig. 9. The profile line of decomposed results in the noisy case. (a) The profile lines of water-based material results; (b) The profile lines of bone-based material results; (c) and (d) are the SSIM and RMSE of water-based and bone-based material images in AR-PPCT.

Fig. 10. The physical and facility photos. (a) The physical object of real experiment 1 in BSRF; (b) The facility of BSRF; (c) The physical object of real experiment 2 in SSRF.

Fig. 11. Projections results. (a), (b) and (c) are the retrieved absorption maps of Born approximation with single ODD method, Linear method and AR-PPCT, respectively; (d), (e) and (f) are the retrieved phase maps of Born approximation with single ODD method, Linear method and AR-PPCT, respectively; (g) and (h) are the profile lines of absorption and phase maps, respectively.

Fig. 12. Tomography results. (a) The $\beta$ image of Born approximation with single ODD method; (c) The $\beta$ image of Linear method; (e) The $\beta$ image of AR-PPCT; (g) The profiles of $\beta$ images; (b), (d) and (f) are the $\delta$ image of Born approximation with single ODD method, Linear method and AR-PPCT, respectively; (h) The profile lines of $\delta$ images.

with an external diameter of 10.7 mm, then injected with water to form the whole sample.

In this experiment, we used water and PTFE as substrates to perform AR-PPCT, MD-SPBI, Linear method and Born approximation with single ODD. Those retrieved projections are shown in Fig. 15. Fig. 16 shows the $\beta$ and $\delta$ images of those methods. The outer ring in the image represents the polyethylene plastic container. There are three different components in the inner ring, namely, three circles with different gray levels in the middle of the ring, LDPE phantom with the lowest gray level on the left, PTFE phantom with the highest gray level at the top, PMMA phantom at the upper right and water at the rest. Fig. 16(g), (h) show the profiles of the $\beta$ and $\delta$ tomographies.
IV. DISCUSSION

In experiments, we compared AR-PPCT with three other quantitative methods, including the phase and absorption projection map, tomographic results of $\beta$ and $\delta$, and base material results. Remarkably, the results of material decomposition in AR-PPCT are better than those of the three comparative methods. It is because there is a single fixed ratio between the information of phase shift and attenuation in Born approximation with single ODD, and it is hard to register two sets of data under different energies in MD-SPBI when the imaging system and the imaged object are mechanically unstable. There are artifacts and noise in the attenuation and material tomography in real experiments due to the lack of feedback and correction from origin data in the Linear method.

In AR-PPCT, since the Fresnel propagator is a Gaussian-like function, the convolution operation indicates it plays a role in spreading and smoothing the wavefront in the evolution process. With feedback and corrections in this iterative method, the noise can be effectively restrained. Here we only focus on reconstruction based on the imaging model without constraints. Reconstruction algorithms based on optimized models can also

from orange squares. Fig. 17 shows the decomposition results of different methods. Comparing the decomposition results of AR-PPCT, MD-SPBI, Linear method and Born approximation with single ODD methods, the most obvious finding was that AR-PPCT method has better material quantitation performance. As shown in Fig. 18, those are the profiles of the water and PTFE images from the orange squares in Fig. 17. These results provide important proof for the decomposition ability of materials in AR-PPCT.

AR-PPCT are better than those of the three comparative methods. It is because there is a single fixed ratio between the information of phase shift and attenuation in Born approximation with single ODD, and it is hard to register two sets of data under different energies in MD-SPBI when the imaging system and the imaged object are mechanically unstable. There are artifacts and noise in the attenuation and material tomography in real experiments due to the lack of feedback and correction from origin data in the Linear method.

In AR-PPCT, since the Fresnel propagator is a Gaussian-like function, the convolution operation indicates it plays a role in spreading and smoothing the wavefront in the evolution process. With feedback and corrections in this iterative method, the noise can be effectively restrained. Here we only focus on reconstruction based on the imaging model without constraints. Reconstruction algorithms based on optimized models can also
be considered by imposing some constraints on the image to reduce artifacts and noise. By calculating the equivalent atomic number \((Z)\), there is an obvious difference between AR-PPCT and other methods. The results of AR-PPCT are very close to the theoretical value, by calculating the relative error, it can get the accuracy is greater than 97.2%. The improved approximation \(\delta = a * \beta + b\) plays a crucial role in this quantitation method.

Unlike dual-energy CT and grating-based imaging, AR-PPCT can effectively distinguish low-Z materials with one set of projection data. Besides, it is easy to implement since there is no additional requirement of optical components, such as gratings or special detectors (PCD) in the beam. The proposed method is better suitable for thin samples in this paper due to its reliance on Born approximation. However, it is the linear approximation of the real and imaginary components of the refractive index and the one-step concept that are not restricted by the sample size. They can be combined with other imaging methods that work well with thick samples to achieve high-quality quantitative imaging. Validation and comparison in the polychromatic laboratory X-ray source are beyond the scope of this study and will be investigated in the future.

The linear relationship in AR-PPCT is a preliminary approximation, which cannot be accurately fitted to more than two base materials at a time. We also assume that \(\delta = a_2\beta^2 + a_1\beta + a_0\), which means that the case of \(N = 2\) in Eq. (8). One of the obstacles is that it is hard to deal with the constant term \(-2\pi \int a_0 dl\). Even if the constant term is eliminated, the equation will also become difficult to solve for the residual term \(\text{Re}\psi_r - \text{Re}\psi_r^{(m)}\).

Therefore, achieving higher precision multi-substrates phase retrieval is a potential research effort.

**V. Conclusion**

In this paper, we propose a one-step method based on the Fresnel diffraction imaging model to perform noise suppression
and material quantitation. This method can reconstruct simultaneously the images of the \( \beta \) and \( \delta \) from original data, and utilize an improved additional approximation to obtain material decomposition results. Both simulation and real experiments have verified that AR-PPCT outperforms the other quantitative methods in noise suppression and material decomposition. Moreover, compared to multi-scanning methods, AR-PPCT reduces the data acquisition time and processing difficulty. Therefore, we anticipate that this algorithm has the potential for biomedical quantitative imaging research, especially imaging for live samples such as insects, mice, and human breast preclinical studies.

APPENDIX

DERIVATION OF THE ITERATIVE ALGORITHM

For convenience, we analyze the situation of 2-dimensional samples here, and this method is also applicable to 3-dimensional samples. Utilizing the linear relation Eq. (9), we can obtain:

\[
\text{Im}\psi_0 = a\text{Re}\psi_0 + \mathcal{F}\left[-k \int b dl\right],
\]

(21)

Substituting the above formula into Eq. (12)

\[
\mathcal{F}\left[\frac{I_z}{I_0} - 1\right] = 2\cos(z\rho^2)\text{Re}\psi_0 + 2a * \sin(z\rho^2)\text{Re}\psi_0
\]

\[
+ 2\sin(z\rho^2)\mathcal{F}\left[-k \int b dl\right],
\]

(22)

The intensity residual of the m-th iteration at projection angle \( \varphi \) is:

\[
\text{Re}\varphi(m) = I_z - h_z \otimes \left[a_n \exp\left(-\frac{M\varphi(m)}{2} + \text{i}\Phi\varphi(m)\right)\right]^2,
\]

(23)

\[
\mathcal{F}(\text{Re}\varphi(m)) = \mathcal{F}\left(\frac{I_z - I_z^\varphi(m)}{I_z^\varphi(m)}\right)
\]

\[
= \left[2\cos(z\rho^2) + 2a \sin(z\rho^2)\right] \left(\text{Re}\psi^\varphi - \text{Re}\psi^\varphi(m)\right),
\]

(24)

The absorption residual of the m-th iteration at projection angle \( \varphi \) is:

\[
\text{Re}\psi^\varphi - \text{Re}\psi^\varphi(m) = \frac{\mathcal{F}(\text{Re}\varphi(m))}{\cos(z\rho^2) + \sin(z\rho^2) * a},
\]

(25)

Then we combine the residual with SART to get its iterative format.

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