Numerical Modeling and Experiment for Single Grid-Based Phase-Contrast X-Ray Imaging

Hyunwoo Lim*, Hunwoo Lee*, Hyosung Cho*, Changwoo Seo*, Soojeul Lee†, Byunggyu Chae†

*Department of Radiation Convergence Engineering, Yonsei University, Wonju, †Bio-Medical IT Convergence Research Division, ETRI, Daejeon, Korea

In this work, we investigated the recently proposed phase-contrast x-ray imaging (PCXI) technique, the so-called single grid-based PCXI, which has great simplicity and minimal requirements on the setup alignment. It allows for imaging of smaller features and variations in the examined sample than conventional attenuation-based x-ray imaging with lower x-ray dose. We performed a systematic simulation using a simulation platform developed by us to investigate the image characteristics. We also performed a preliminary PCXI experiment using an established a table-top setup to demonstrate the performance of the simulation platform. The system consists of an x-ray tube (50 kV, 5 mAs), a focused-linear grid (200-lines/inch), and a flat-panel detector (48-mm pixel size). According to our results, the simulated contrast of phase images was much enhanced, compared to that of the absorption images. The scattering length scale estimated for a given simulation condition was about 117 nm. It was very similar, at least qualitatively, to the experimental contrast, which demonstrates the performance of the simulation platform. We also found that the level of the phase gradient of oriented structures strongly depended on the orientation of the structure relative to that of linear grids.

Keywords: Phase-contrast x-ray image, Simulation platform, X-ray grid, Image contrast

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based PCXI, which has great simplicity and minimal requirements on the setup alignment. The information of the phase shift can be extracted by using Fourier processing. We developed a useful simulation platform for PCXI and performed a systematic simulation to investigate the image characteristics. We also performed a preliminary PCXI experiment using an established table-top setup to demonstrate the performance of the simulation platform. In the following sections, we briefly describe the numerical modeling of the PCXI used in the simulation platform and present the results.

Materials and Methods

1. Numerical modeling for single grid-based PCXI

Fig. 1 shows the schematic illustration of a single grid-based PCXI setup in which an x-ray grid is placed midway between the x-ray source and the detector and a sample is placed ahead of the grid. As illustrated in Fig. 1, when x-rays from the source pass through a sample, the wavefront of the transmitted x-rays is distorted by the refraction of the x-rays due to the difference in the refractive indexes of the sample structures and its intensity is modulated by the periodic x-ray grid strips.

In x-ray physics, image contrast is generated due to the difference in complex refractive index $n$ of the sample and described as follows:

$$n(x,y,z) = 1 - \delta(x,y,z) + i\beta(x,y,z),$$  \hspace{1cm} (1)

where $\delta$ is the decrement of the real part of the refractive index responsible for phase shift of the x-rays and the imaginary part $\beta$ describes the absorption index. When x-rays pass through a sample, not only their amplitude but their phase is altered as well. Because x-rays are a form of high-energy lights, they can be treated as electromagnetic waves and their propagation is described by the Helmholtz equation, assuming that monochromatic x-rays are propagated through free space:

$$\nabla^2 \psi(r) + k^2 \psi(r) = 0,$$

where $V^2$ is the Laplacian operator, $\psi$ is a scalar wave function, $k$ is the wave number, $\omega$ is the angular frequency, and $c$ is the speed of light in vacuum. Fig. 2 shows the schematic illustration of a geometry for the free-space propagation of x-rays. The wavefront $\psi(x,y,z)$ in the detector plane is calculated using the Huygens-Fresnel principle:

$$\psi(x,y,z) = \frac{1}{i\lambda} \int_0^\infty \int_0^\infty \psi(x',y',0) \frac{e^{i(kr - \omega t)}}{r} dxdy,$$

where $\lambda$ is the wavelength of the x-rays, $r$ is the distance between points in the sample and detector planes, $\theta$ is the angle illustrated in Fig. 2, and $A$ is the wave amplitude. Assuming small diffraction angles (i.e., $\cos \theta \approx 1$) and $r \approx z$

Eq. (3) can be written as:

$$\psi(x',y',0) = A e^{-i(kr - \omega t)} e^{i(kr - \omega t)},$$

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Eq. (3) can be written as:
Neglecting the constant phase term $e^{ikz}$, Eq. (4) can also be expressed as the convolution with the propagation kernel, $h(x,y)$, as follows:

$$
\psi(x, y) = \psi(x, y, 0) \otimes h(x, y),
$$

(5)

where $\otimes \otimes$ indicates the two-dimensional (2D) convolution operator. In addition, considering the system response function (SRF), the image intensity of the sample, $I$, can be expressed as:

$$
I = [\psi(x, y)]^0 \otimes \otimes SRF.
$$

(6)

To model an x-ray grid, we considered an ideal linear grid in which the absorption by any interspace material is ignored. Fig. 3 shows the primary transmission, $t_{grid}$, of an ideal linear grid oriented in the vertical direction. It can be expressed mathematically as a one-dimensional (1D) square function using a Fourier series:

$$
t_{grid}(x) = \sum_{n=-\infty}^{\infty} \frac{d}{P} \text{sinc} \left( \frac{m n}{P} \right) \left( \frac{2m}{P} \right),
$$

(7)

where $P$ is the grid pitch and $d$ is the width of the lead strips. Thus, the image intensity of the sample with a linear grid, $f_{sg}$, can be expressed as:

$$
f_{sg} = I \times t_{grid}(x).
$$

(8)

The analysis of the phase shift in PCXI is described in detail in Ref. The two raw images of the sample with grid ($f_{sg}$) and the bare grid ($f_b$) are acquired separately and Fourier-transformed. In the Fourier domain, the areas surrounding the primary and the first harmonic peaks are selected using a band-pass filter separately and then inverse Fourier-transformed to yield the primary image ($\tilde{f}_{0,s}$), i.e., retrieved absorption image, and the first harmonic image ($\tilde{f}_{1,s}$) of the sample by normalizing with the bare grid images as:
\[ f_{V} = \frac{f_{1,s}}{f_{0,s}} \]  

(10)

where \( f_{0,s} \) and \( f_{1,s} \) are the primary and first harmonic images of the sample with grid, respectively, while \( f_{0,g} \) and \( f_{1,g} \) are those of bare grid. To extract gradient phase information, the ratio of \( f_{1,s} \) and \( f_{0,s} \) is taken as:

\[ \frac{f_{1,s}}{f_{0,s}} = \frac{F_{1,s}}{F_{0,s}} \]

(9)

Fig. 4 shows the simplified Fourier processing in the single grid-based PCXI to extract absorption image and differential phase image from the two raw images of the sample with grid (\( f_{0,s} \)) and the bare grid (\( f_{0,g} \)).

The intensity of the phase image depends on the x-ray wavelength (\( \lambda \)), the grid period (\( p \)), and the system geometry. The size of the sample structure whose phase

Fig. 4. The simplified Fourier processing in the single grid-based PCXI to extract absorption image and differential phase image from the two raw images of the sample with a linear grid (\( f_{0,s} \)) and the bare grid (\( f_{0,g} \)).

Fig. 5. (a) The 3D numerical chest phantom (478x258x434 voxels) in AP positioning (left) and LA (right) positioning and (b) the 3D Shepp-Logan phantom (400x400x400 voxels) used in the simulation.
information can be appreciably detected is known to be limited to an upper threshold size,\(^{(10)}\) which is defined as the scattering length scale \((L)\):

\[
L = \frac{(SDD - SOD) \cdot (SDD - GDD) \lambda}{p},
\]

(11)

where \(SDD\), \(SOD\), and \(GDD\) is the source-to-detector distance, the source-to-object distance, and the grid-to-

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**Table 1.** Imaging acquisition conditions used in the simulation and the experiment.

| Parameter                        | Dimension               |
|----------------------------------|-------------------------|
| Source-to-object distance (SOD)  | 80 cm                   |
| Object-to-grid distance (OGD)    | 20 cm                   |
| Grid-to-detector distance (GDD)  | 100 cm                  |
| Grid strip density               | 200 lines/inch          |
| Grid focal distance              | 100 cm                  |
| Detector pixel size              | 48 \(\mu\)m             |
| Focal spot size                  | 0.1 mm                  |
| Tube voltage                     | 50 kV (monochromatic in simulation) |
|                                  | 50 kV\(_p\) (polychromatic in experiment) |
| Sample                           | Chest, Shepp-Logan (simulation) |
|                                  | Animal bone, chicken wing (experiment) |

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**Fig. 6.** Table-top setup established for the experiment. It consists of an x-ray tube (100-\(\mu\)m focal spot size), a focused-linear grid (200-lines/inch strip density), and a CMOS-type flat-panel detector (14.5 cm×11.6 cm active area, 48-\(\mu\)m pixel size).

**Fig. 7.** The differential phase images of the chest phantom in AP positioning simulated with a vertical grid (**top right**) and a horizontal grid (**bottom left**) and their combined image (**bottom right**). The retrieved absorption image (**top left**) is also indicated as the reference.
detector distance, respectively. The larger the scattering length scale, the larger the phase signal.

2. Simulation and experimental setup

We developed a useful simulation platform based on the above descriptions for PCXI study. Fig. 5 shows (a) the three-dimensional (3D) numerical chest phantom (478×258×434 voxels) in anterior-posterior (AP) positioning (left) and lateral (LA) positioning (right) and (b) the 3D Shepp-Logan phantom\(^\text{12}\) (400×400×400 voxels) used in the simulation. The chest phantom, originally produced by authors at the University of Pernambuco in Brazil,\(^\text{13}\) was defined by us with proper complex refractive indexes by segmentation into several compartments representing skin, muscle, bone, lung, fat, water, soft tissue, etc.\(^\text{14}\) In the simulation, monochromatic x-rays of 50 keV were used and the strip density of the used grid was 200 lines/inch. The corresponding wavelength of the x-rays and the grid period were about \(\lambda=0.25\) Å and \(p=127\) µm, respectively. SDD=200 cm, SOD=80 cm, and GDD=100 cm were used. The scattering length scale estimated for the given simulation condition was about 117 nm. The detailed conditions used in the simulation and experiment are listed in Table 1.

Fig. 6 shows the table-top setup established for the PCXI experiment. It consists of an x-ray tube (100-µm focal spot size, Oxford Ins., TF5011), a focused-linear grid (200-lines/inch strip density, JPI Healthcare Corp.), and a CMOS-type flat-panel detector having an active area of 14.5 cm×11.6 cm (48-µm pixel size, Rayence Corp., Xmaru1215). The same system geometry used in the simulation was applied in the experiment. More details of the experimental procedure can be found in our previous paper.\(^\text{15}\)

![Absorption](image1.png) ![Differential phase](image2.png)

**Results and Discussion**

Fig. 7 shows the differential phase images of the chest phantom in AP positioning simulated with a vertical grid (top right) and a horizontal grid (bottom left) and their combined image (bottom right). The retrieved absorption image (top left) is also indicated as the reference. As indicated in Fig. 7, the contrast of the phase images was, as expected, much higher than that of the absorption images.

In addition, a linear grid can detect phase gradient in only one direction perpendicular to the grid strips. Note that the segments of the structure boundary perpendicular to the grid direction are more highlighted in the differential phase images (see the spine and the clavicle for vertical grid and horizontal grid marked by arrows in Fig. 7, and vice versa). The level of the phase gradient of oriented structures depends on the orientation of the structure relative to that of linear grids.

One possible solution to the orientation problem of a linear grid is to employ more sophisticated grids such as crossed grids that consist of square cells to enable imaging...
of phase gradient in multiple directions with a single exposure. Kottler et al.\textsuperscript{16} showed that measurements in two orthogonal directions are often necessary to improve visibility and reduce artifacts in the image. Wen et al.\textsuperscript{17} recently described an x-ray differential phase-contrast imaging method based on 2D transmission gratings that were directly resolved by an x-ray detector and quantified the effects of x-ray refraction and diffraction in the sample through spatial harmonic analysis. The use of 2D gratings allows differential phase contrast in several directions to be obtained from a single image, which obviates the need for multiple exposures and separate measurements for different directions. In the study, instead, as indicated in Fig. 7, we simply summed the two retrieved differential phase images with a vertical grid and a horizontal grid, which gives phase gradient in a direction at 45 degrees to both the x and y directions.\textsuperscript{18} See the spine and the clavicle in the combined differential image marked by arrows in Fig. 7. Fig. 8 shows similar phase images of the chest phantom in LA positioning; see also the body of humerus and the ribcage indicated by arrows in Fig. 8.
For more quantitative analysis of the image characteristics of PCXI, we repeated the same simulation procedure using the 3D Shepp-Logan phantom. Fig. 9 shows the differential phase images of the Shepp-Logan phantom simulated with a vertical grid (top right) and a horizontal grid (bottom left) and their combined image (bottom right). Fig. 10 shows the intensity profiles measured along the line segments $\overline{AB}$ indicated in Fig. 9 for the differential phase image and the absorption image. As indicated in Fig. 10, the vertical grid emphasizes vertical edges by a horizontal gradient, detecting small features and variations in the sample that was not clearly visible in the absorption image (see the intensity variations marked by arrows).

Fig. 11 shows complete sets of the PCXI results retrieved from a single raw image of (a) animal bone and (b) chicken wing with a 200-lines/inch vertical grid obtained at the given x-ray tube conditions of 50 kV$_p$ and 5 mAs. The image contrast of the phase images was much enhanced, compared to that of the absorption images, and was similar, at least qualitatively, to the simulated contrast, indicating the performance of the developed simulation platform.

**Conclusion**

We successfully obtained phase-contrast x-ray images of much enhanced contrast, compared to conventional attenuation-based images, by using the single grid-based technique from both the simulation and experiment. The simulated contrast of the phase images was similar, at least qualitatively, to the experimental contrast, which demonstrates the performance of the developed simulation platform. The scattering length scale estimated for a given simulation condition was about 117 nm. Consequently, the simulation platform worked properly and demonstrated that the single grid-based approach seemed a useful method for PCXI with great simplicity and minimal requirements on the setup alignment. We expect that the simulation platform developed in this work will be useful for designing optimal PCXI systems. More quantitative evaluation of the image characteristics will be performed soon.
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Conflicts of Interest

The authors have nothing to disclose.

Availability of Data and Materials

All relevant data are within the paper and its Supporting Information files.

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