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Novel Detection Scheme for X-ray Small-Angle Scattering

Guang Li,

Biomedical Imaging Center, BME/CBIS, Rensselaer Polytechnic Institute, New York, USA

Wenxiang Cong,

Biomedical Imaging Center, BME/CBIS, Rensselaer Polytechnic Institute, New York, USA

James S. Michaelson,

Department of Pathology, Harvard Medical School, Massachusetts, USA

Hong Liu,

Center for advanced medical imaging, University of Oklahoma, USA

Lars Gjestebj, and

Biomedical Imaging Center, BME/CBIS, Rensselaer Polytechnic Institute, New York, USA

Ge Wang, Fellow, IEEE

Biomedical Imaging Center, BME/CBIS, Rensselaer Polytechnic Institute, New York, USA

Abstract

X-ray imaging techniques, including x-ray radiography and computed tomography, have been in use for decades and proven effective and indispensable in diagnosis and therapy due to their fine resolution and fast acquisition speed. However, the innate disadvantage of x-ray is the poor soft tissue contrast. Small-angle scattering signals were shown to provide unique information about the abnormality of soft tissues that is complementary to the traditional attenuation image. Currently, there is no effective small-angle scattering detection system. In this paper, we propose a new “collimation” design dedicated to capture a small-angle scattering radiographic image directly, which carries critical pathological information for differentiation between normal and abnormal tissues. Our design consists of two interlaced gratings so that both the primary flux and Compton scattering photons are effectively blocked to leave the apertures mainly open to small-angle scattering photons. Theoretical analysis and Monte Carlo simulations demonstrate that small-angle scattering radiography is feasible with our proposed technology.

Index Terms

Small-angle scattering; grating based x-ray imaging; pathological studies

I. Introduction

Recent developments of x-ray imaging hardware have greatly improved spatial resolution, temporal resolution, and image contrast in x-ray radiography and computed tomography

(CT). Specifically, x-ray sources with higher flux and smaller focal spot deliver higher spatial resolution, novel x-ray detectors provide high signal-to-noise ratio and spectral information, and advanced mechanical components enable unprecedented speed, precision, and stability in positioning x-ray components. Also, novel x-ray imaging modes emerged in the past several years and were successfully put to use in preclinical research [1], [2], [3], [4], [5]. With the improved performance of x-ray imaging techniques, new applications were explored; for example, micro-CT was recently employed to image cancer specimens and test their margin positivity. Of course, x-ray imaging still has much room for improvement. Its poor soft tissue contrast is due to x-ray attenuation coefficients roughly proportional to the fourth power of atomic number [6], and biological soft tissues are rather similar in their compositions of chemical elements. To address this challenge, researchers have been investigating alternative contrast mechanisms to reveal soft tissue features. One popular option to improve contrast resolution is to introduce high-Z contrast agents. Unfortunately, there are many cases in which a contrast agent is not easy to reach the target area and take effect, such as for in vitro cancer specimen imaging. The emergence of Talbot interferometers [7], with synchrotron and micro-focus x-ray sources, and Talbot-Lau interferometers [8] with hospital-grade x-ray sources, has enabled acquisition of both the traditional attenuation image and the differential phase and small-angle scattering images, which offer better contrast for low density materials such as soft tissues. Also, a recently emerging single shot method [9], [10] works as a simplified phase-retrieval method to obtain differential phase images.

Small-angle scattering or dark field imaging is particularly important for extraction of microstructural features, directly relevant to cancer imaging. It is reported that small-angle scattering signals contain critical information complementary to that in the attenuation and phase-contrast images. A large body of literature demonstrates that small-angle scattering imaging provides positive correlation with the presence of breast cancer [11], [12], [13], and different tissues have quite distinct coherent scattering profiles [14], and distinct scattering peaks [9]. For example, scattering profiles from normal tissues have a sharper peak at position $x = 0.11^\circ A^{-1}$, which indicates the presence of adipose component [15], the scattering profiles from malignant tissues present a broad scattering peak at $x = 0.17^\circ A^{-1}$ [16], and the scattering peaks from fibrous collagens are positively related to fibril stacking period and collagen fiber alignment [17]. Nevertheless, the small-angle scattering or dark field information obtained using the Talbot or Talbot-Lau methods is a mixed signal, in which we do not know precisely the angular information in the scattering data, and therefore the method is referred to as indirect.

Direct coherent scattering systems [18], [19], [20] have great potential to distinguish subtleties between different tissues due to angular sensitivity. Current scattering-based imaging techniques perform slot scanning aided by a collimated detector. These systems collect scattering signals at characteristic angles and obtain a 2D material map point-by-point or line-by-line which is time consuming, especially when small-angle scatter tomography is needed. Meanwhile, as we all know, the small-angle scattering from one point is radially symmetric, but in the associated imaging geometry, the collimated detector is usually deviated from the direction along which the primary x-ray travels to obtain the

small-angle scattering signal from only one direction, and thus a lot of useful small-angle scattering signals are discarded and wasted.

In this paper, we proposed a completely new small-angle scattering imaging system which can detect the small-angle scattering signals effectively and efficiently. The dedicated small-angle scattering imaging scheme is composed of two interlaced gratings. The key idea behind our design is that both the primary x-rays and Compton scattering photons are basically blocked so that only small-angle scattering x-rays are admitted to go through the paired gratings and reach the detector behind the gratings. In the rest of this paper, we first describe the theory and method in the second section. Then, we report our numerical results using the parallel beam geometry in the third section. Finally, we discuss relevant issues and conclude the paper.

II. METHODS

A. Small-Angle Scattering Principle

When x-rays pass through a volume element in an object, the scattering process can be illustrated as in Fig. 1. From [21], the scattered photon count from this point can be expressed as

$$dI_{scat}(E, \theta) = I_0(E) dV \frac{r_e^2}{2} (1 + \cos^2 \theta) f(\vec{x}, q_\theta), \quad (1)$$

where $I_0(E)$ is the number of incident x-ray photons with energy E per unit area, dV is the volume element, r_e is the classical electron radius, θ is the scatter angle, $f(\vec{x}, q_\theta)$ is the scatter factor at location $\vec{x} = (x, y, z)$, and q_θ is the momentum transfer which can be written as

$$q_\theta = \frac{E \sin(\theta/2)}{hc}, \quad (2)$$

with h being the Planck constant and c being the speed of light. Combining (1) and (2), the general formula of the total scatter irradiance detected at the pixel $\vec{x}_d$ on the detector can be derived as

$$I_{scat}(E, \vec{x}) = \int_V \int_q \int_\Omega I_0(E, \vec{x}) \frac{r_e^2}{2} (1 + \cos^2 \theta) \delta f(\vec{x}, q) d\Omega dq dV \quad (3)$$

where $\delta = \delta(q - \frac{E \sin(\theta/2)}{hc})$ and Ω is the solid angle covered by one pixel of the detector.

In the traditional slit-based geometry, the detection procedure was simplified to detect one single scattering angle for even one single voxel, and it was easy to estimate the scatter factor, but the imaging process is time-consuming. What we want to do here is to construct a new setup that can effectively and efficiently capture small-angle scattering signals.

B. System Design

As our proposed small-angle scattering imaging scheme is new, we start with the parallel beam geometry to verify the feasibility. In the parallel-beam geometry, the schematic system design is illustrated in Fig. 2. The most important component in this system is the combination of two absorption gratings (red columns in Fig. 2) made of tungsten or lead. The duty cycle of each grating is 50%. The two gratings are complementary, and all the primary parallel x-rays are completely blocked. Only those rays that pass through the object and scatter at small/specific angles can be detected by the detector behind the gratings. Between the two layers, the gap can be used to modulate the incidence angle.

C. System Analysis

Scattered photons are often considered as noise in practice as they randomly diffuse over the field of view, and cannot be effectively analyzed or removed. Here our proposed detection scheme can specifically extract small-angle scattering signals with appropriate geometrical parameters. All the key parameters are shown in Fig. 3. Each structural unit of the grating contains two parts: solid cell (each red component in Fig. 3) and hollow cell. The height and width of each unit are h_1 and $2w_1$ respectively, and the widths of the solid cell and the hollow cell are all equal to w_1 . The length of the gap between two layers is l_1 . In order to determine these parameters optimally, we first set up a rectangular coordinate system as shown in Fig. 3. For a scattered photon from a point $O = (x, y)$ to reach a point $p_o = (a, 0)$ on the detector, it must go through the three surfaces shown in Fig. 3 without being attenuated by the grating metal. Hence, the following four equations should be simultaneously satisfied:

$$\begin{cases} -\frac{w_1}{2} < a + \frac{(2h_1 + l_1)(x - a)}{y} < \frac{w_1}{2}, \\ -\frac{w_1}{2} < a + \frac{(h_1 + l_1)(x - a)}{y} < \frac{w_1}{2}, \\ \frac{w_1}{2} < a + \frac{h_1(x - a)}{y} < \frac{3w_1}{2}, \\ \frac{w_1}{2} < a < \frac{3w_1}{2}. \end{cases} \quad (4)$$

Here is an explanation of (4): The first to third equation respectively means that a scattered photon from point $O = (x, y)$ can pass through the third to first surface, and the fourth equation means that the photon can successfully reach the detector. By simplifying (4), we can draw the conclusion that if $a > h_1 w_1 / (h_1 + l_1) + w_1/2$, the following relationship must hold

$$\frac{-\frac{w_1}{2} - a}{2h_1 + l_1}y + a < x < \frac{\frac{w_1}{2} - a}{h_1 + l_1}y + a. \quad (5)$$

Otherwise, we have

$$\frac{\frac{w_1}{2} - a}{h_1}y + a < x < \frac{\frac{w_1}{2} - a}{h_1 + l_1}y + a. \quad (6)$$

From (5) and (6), we can derive the angular range for scattering signals to arrive at $p_o = (a, 0)$:

$$\arctan \frac{a - \frac{w_1}{2}}{h_1 + l_1} < \theta(a) < \arctan \frac{a + \frac{w_1}{2}}{2h_1 + l_1} \quad (7)$$

or

$$\arctan \frac{a - \frac{w_1}{2}}{h_1 + l_1} < \theta(a) < \arctan \frac{a - \frac{w_1}{2}}{h_1} \quad (8)$$

which means the angular range at point p_o is directly related to its location. In the above equations, the height h_1 of the grating is inversely proportional to the density of the material. In practice, h_1 must be large enough to block all the primary beam, and it is typically dozens of micrometers. When gap length l_1 is much larger than height h_1 , most of the points in the range $(w_1/2, 3w_1/2)$ will satisfy (5) and (7), otherwise it is the opposite. As the scattering angle ought to be quite small, (7) and (8) can be simplified as follows:

$$\frac{a - \frac{w_1}{2}}{h_1 + l_1} < \theta(a) < \frac{a + \frac{w_1}{2}}{2h_1 + l_1}, \quad (9)$$

$$\frac{a - \frac{w_1}{2}}{h_1 + l_1} < \theta(a) < \frac{a - \frac{w_1}{2}}{h_1}. \quad (10)$$

Let $\frac{h_1}{h_1 + l_1}$ be k_1 , the energy distribution function $E(\theta')$ can be defined as

$$\begin{aligned} E(\theta') &= \int_{w_1/2}^{3w_1/2} T(a) da \\ &= \int_{w_1/2}^{w_1/2 + k_1 w_1} T(a) da + \int_{w_1/2 + k_1 w_1}^{3w_1/2} T(a) da. \end{aligned} \quad (11)$$

In (11), $\theta' = \tau(h_1 + l_1)$, $\in (0, 2w_1(h_1 + l_1)/(2h_1 + l_1))$ and $T(a)$ can be written as

$$T(a) = \begin{cases} 1 & \theta' \in \theta(a) \\ 0 & \theta' \notin \theta(a) \end{cases} \quad (12)$$

The first item in the rightmost side of (11) can be noted as

$$\begin{aligned} E_1(\theta') &= \int_{w_1/2}^{w_1/2 + k_1 w_1} Q(t_1) - Q(t_2) da \\ &= \int_{w_1/2 + k_1 \tau}^{w_1/2 + k_1 w_1} da - \int_{\tau + w_1/2\delta\tau < k_1 w_1}^{w_1/2 + k_1 w_1} da \end{aligned} \quad (13)$$

where $t_1 = a = (-\frac{w_1}{2} + k_1 \tau)$, $t_2 = a - (\tau + \frac{w_1}{2})$, and the second term can be written as

$$\begin{aligned} E_2(\theta') &= \int_{w_1/2 + k_1 w_1}^{3w_1/2} Q(t_3) - Q(t_4) da \\ &= \int_{k_2}^{3w_1/2} da - \int_{\tau + \frac{w_1}{2} \& \tau < w_1}^{3w_1/2} da \end{aligned} \quad (14)$$

where $k_2 = \min(w_1/2 + k_1 w_1, (1 + k_1)\tau - w_1/2)$, $t_3 = a - ((1 + k_1)\tau - w_1/2)$, $t_4 = a - (\tau + w_1/2)$. In (13) and (14), Q is a step function whose value is equal to 1 when its argument is greater

than zero; otherwise, is equal to 0. Combining (13) and (14), we can draw the following conclusion

$$E(\theta') = E\left(\frac{\tau}{h_1 + l_1}\right) \quad (15)$$

$$= \begin{cases} (1 - k_1)\tau & 0 \leq \tau < w_1 \\ (1 - k_1)w_1 & \tau = w_1 \\ 2w_1 - (1 + k_1)\tau & w_1 < \tau \leq \frac{2(h_1 + l_1)}{2h_1 + l_1}w_1 \end{cases}$$

From (15), it is seen that the acquired small-angle scattered photons from different angles approximately form a triangular distribution. We define the principal angle as

$$\theta_p = \frac{w_1}{h_1 + l_1} \quad (16)$$

around which small-angle scattered photons come to the detector element. Equation (15) is a standard triangular distribution. The range of distribution depends on the ratio of w_1 to $w_1 + l_1$. Given a specific scattering angle, the relationship between the geometry parameters can be determined according to (15). As the scheme shown in Fig. 2 is of left-right symmetry, the energy distribution function $E(\theta')$ should be an even function which means it can be modified as

$$E(\theta') = E\left(\frac{\tau}{h_1 + l_1}\right) \quad (17)$$

$$= \begin{cases} (1 - k_1) |\tau| & 0 \leq |\tau| < w_1 \\ (1 - k_1) w_1 & |\tau| = w_1 \\ 2w_1 - (1 + k_1) |\tau| & w_1 < |\tau| \leq \frac{2(h_1 + l_1)}{2h_1 + l_1}w_1 \end{cases}$$

Equation (17) can be treated as a response function of the proposed system. Assuming that the scatter factor from a position $M = (x, z)$ along a direction θ is $f(M, \theta)$, and if we ignore the absorption for the scattering signal when it passes through the sample, the captured scattering signal can be represented as the following based on (1):

$$F(x') = \sum_z \sum_x f(x, z, \theta) E(\theta) \big|_{x' = x \pm z\theta} \quad (18)$$

In order to explain what the physical meaning is in (18) more intuitively, let us simply assume that most of the energy is captured around the principal angle. We have

$$F(x') = c \sum_z f(x, z, \theta_p) \big|_{x' = x \pm z\theta_p} \quad (19)$$

where c is a constant. Equation (19) means the signal from one point is transformed to two symmetrical points with respect to this point. Based on this derivation, we can use a two-dimensional small-angle scattering imaging grating which is composed of a pair of two-dimensional checkerboard-like gratings as shown in Fig. (4). The image generation function in the two-dimensional case can be represented as

$$F(x', y') = \sum_{z, x, y} f(x, y, z, \theta) E(\theta) \big|_{\sqrt{x'^2 + y'^2} = \sqrt{x^2 + y^2} \pm z\theta} \quad (20)$$

Using the same assumption, (20) can be simplified as

$$F(x', y') = c \sum_z f(x, y, z, \theta_p) \big|_{\sqrt{x'^2 + y'^2} = \sqrt{x^2 + y^2} \pm z\theta_p} \quad (21)$$

Unlike in the one-dimensional case where the scattering signal from one point is converted to two points, in the two-dimensional case, the scattering signal from one point is converted to four sides or approximately a circle of radius $z\theta_p$. The following simulation experiments were all based on the use of a two-dimensional grating. We used the EGSnrc simulation system for Monte Carlo simulation to verify the feasibility of the proposed small-angle scattering imaging scheme.

III. Results

EGSnrc is a well-known simulation software whose function is to model the propagation of electrons and photons through matter. Because it relies on Monte Carlo simulation, it is highly accurate and can be used to validate the feasibility of our proposed detection scheme. Common scattering contains Compton scattering and Rayleigh scattering. According to the instruction of EGSnrc software, it is known that this software can simulate both Compton and Rayleigh scattering. Rayleigh scattering can be treated as small-angle scattering. Although it cannot simulate the small-angle scattering signals coming from Bragg's

diffraction, the scattering signals from the Rayleigh scattering can also be used to demonstrate the effectiveness of our small-angle scattering signal detection system.

A. System Feasibility

The two simulations in this subsection were used to demonstrate the feasibility of our novel small-angle scattering detection system. The first experiment was performed to prove that our proposed small-angle scattering detection system can be used to capture small-angle scattering signals effectively and efficiently. The second simulation sought to demonstrate that the proposed detection system can differentiate different materials and be applicable to the polychromatic case.

The first simulation was performed in a parallel beam geometry with monochromatic x-ray at 20 keV. The total number of photons was set to 1.0×10^{10} . The detector involved was an ideal detector and hence its height, material, and the scattering events in it would not be considered. It contained 50×50 pixels with a 0.4 mm pixel size, and each pixel covered 16×16 cells of the grating. The paired two-dimensional gratings were made of tungsten. The width and height of each cell was $25 \mu\text{m}$ and $120 \mu\text{m}$, respectively. The gap between the two layers was adjustable and could be used to modify the incident angle of scattering x-rays; it was set to be $280 \mu\text{m}$ in this simulation. To start, no phantom was put in front of the grating, and the x-ray photons traveled directly to the grating. Photons passing through the double gratings and reaching the detector would be collected. In the following step, three square cuboids with the same length and width of 2 mm and different heights of 1 mm, 2 mm, and 4 mm were introduced. These cuboids were made of water and put 2.6 mm, 1.6 mm, and 0.6 mm away from the first layer of the gratings, respectively, to keep the center of them at the same line, which is parallel to the gratings (Fig. 5(a)). The captured scattering images are shown in Fig. 5(b). The left image is the image without a phantom, due to Compton scattering and Rayleigh scattering of the gratings, and we can call it background scattering. The ratio of background scattering counts to primary beam counts was approximately 1/7000. The right image is the image with a phantom put in front of the gratings. From these two images, it is clear that when no phantom is placed in front of the gratings, the background scattering is very smooth and its intensity is very small, which means most of primary beams are blocked and cannot reach the detector. When the phantom is put in front of the grating, three squares with different intensities can be seen in the captured image. By comparing these two images, we can conclude that the formation of the bright squares results from small-angle scattering since the signal intensity is stronger when phantom is placed in front of the gratings. Fig. 5(c) shows the vertical profiles along the central lines of the two images in Fig. 5(b). From Fig. 5(c), we can see that when there is no phantom placed in front of the grating, the background scattering signal coming from the grating is very smooth, and when phantom is placed, the captured scattering signal is much stronger than the background scattering. With the increasing of the phantom height, the signal intensity is getting bigger. By quantitative analysis of the signal intensity, we can prove that these signals come from small-angle scattering. According to the relationship between the incident flux and the small-angle scattering intensity [22]:

$$P_1 = I_0 \sigma(0) t \Omega \exp(-\mu t) \quad (22)$$

where I_0 is the incident flux, $\sigma(0)$ is the scattering coefficient in the forward direction per unit solid angle per unit thickness of sample, t is the sample thickness, and μ is the linear attenuation coefficient, when the x-ray photon energy is 20 keV, the attenuation coefficient for water is 0.8096 cm^{-1} . Based on (22), we can get the ratios of the small-angle scattering signals passing through different heights of water phantoms. The ideal ratio of the signal intensity from 4 mm height of square cuboid to that from 2 mm height of square cuboid should be 1.7. And the ratio of the signal from 2 mm height of square cuboid to 1 mm height of square cuboid should be 1.84. Subtracting the background scattering signal from the small-angle scattering signal from the phantom and averaging the three peaks separately, we can get the average scattering signals of the three square cuboids as 4.395×10^{-7} , 2.641×10^{-7} , and 1.431×10^{-7} . Thus, the corresponding measured ratios are 1.664 and 1.845, which are very similar to the ideal results. This demonstrates that EGSnrc can simulate small-angle scattering and our proposed scheme can effectively collect small-angle scattering signals. Moreover, because we can acquire the whole small-angle scattering image with a single exposure, it is a very efficient detection method.

In the second simulation, the involved phantom contained three square cuboids which are composed of three materials respectively (Fig. 6): water (green), fat (blue) and fibro-glandular tissue (magenta) whose intensity was 1.04 g/cm^{-3} with the mass fraction of carbon, hydrogen, and oxygen being $0.185 : 0.094 : 0.68$ [23]. The dimensions of these square cuboids are all $2 \text{ mm} \times 2 \text{ mm} \times 4 \text{ mm}$. Monochromatic x-rays with 20 keV were first applied to illuminate these samples. In real applications, the commonly used x-ray sources for small-angle scattering detection all have very narrow spectra as the small-angle scattering signals strongly depend on the x-ray wavelength [21], [24]. And hence, in the following simulation, a polychromatic source whose spectrum obeyed a Gaussian distribution with the mean value of 20 keV and the standard deviation of 3 keV was introduced to take place of the former monochromatic source. The left image in Fig. 6(b) is from the monochromatic source and the right one is from the polychromatic source. The vertical central profiles of the two images in Fig. 6(b) are shown in Fig 6(c). Because different energy will bring in different background scattering caused by the gratings, we collected the corresponding backgrounds for different x-ray sources. In order to compare the scattering results from different sources more intuitively, background subtraction should be performed first. After this step, we can get the pure small-angle scattering images from the phantoms. The vertical central profiles of these pure small-angle scattering images are shown in Fig. 6(d), and it can be seen that the polychromatic source makes a small change to the peak values, but the slopes of the peaks are unchanged, which means that the system resolution is invariable with the changing of the energy spectrum of the x-ray source. This is because the incident angle of the detected small-angle scattering signal is independent of x-ray wavelength. From the profiles in Fig. 6(d), we can also see that the scattering intensities for different materials are different. Because the current simulation software can only simulate Rayleigh scattering related to the density, and not the stronger signals from Bragg's

diffraction due to structure information, the differences are not very obvious between these three materials which have similar densities.

B. System Performance

In this subsection, simulations were performed to study the performance of the proposed detection scheme in terms of resolution and quantum detection efficiency. The configuration of the gratings is the same that we used in the first subsection. There were two types of phantoms in the simulation. The first one is shown in the left of Fig. 7(a), which was composed of many concentric cylinders. The solid parts (pink parts) of the phantom were made of water. The hollow parts are air. The solid parts and hollow parts were alternately placed. The radii from the innermost to outermost were 1 mm to 9 mm with a common difference of 1 mm. The second phantom type is shown in Fig. 7(b), which only contained the outermost cylinder from the first phantom. As there were tens of thousands of separate regions involved and the simulation based on EGSnrc was very time-consuming, the grating was not set to the same size as the phantom; it covered the whole phantom in the horizontal direction but only half in the vertical direction. The parallel beam was confined to the same size as the grating.

There were two controls involved. In the first control, the heights of the two phantoms were set to 4 mm and placed 0.5 mm away from the grating. In the second control, the heights of the phantoms were changed to be 10 mm. In order to show the detection quantum efficiency more intuitively, the absorption image of the phantom composed of several concentric cylinders was acquired in another simulation. The collected scattering images in the first and second controls are shown in Fig. 8(a),(c) and the profiles along their respective central vertical lines are shown in Fig. 8(b),(d). The left images in Fig. 8(a),(c) are the scattering images of a phantom composed of concentric cylinders and the right images correspond to the phantom with only the outermost cylinder. From Fig. 8(a),(c), it is intuitive that when the phantom height is 4 mm, the resolution of the detected scattering image is higher, and when phantom height is changed to be 10 mm, the resolution is lower. The neighboring peaks in the red profiles from the concentric cylinder phantom in Fig. 8(b),(d) could overlap to reduce the resolution. If the width of a single peak increases, there will be more overlap between neighboring peaks. We can use full width at half maximum (FWHM) of the gradient profile of the blue profiles in Fig. 8(b),(d) to define the resolution quantitatively. The FWHM values are 1.5 pixels and 3.4 pixels, respectively. As the pixel size of the detector is 0.4 mm, the system resolution in above two cases can be obtained as 0.6 mm and 1.36 mm, respectively.

The absorption image of the phantom composed of several concentric cylinders with the height of 4 mm is as shown in Fig. 9(a), and the profile along its vertical central line is shown in Fig. 9(b). It is evident that the image in Fig. 9(a) is very similar to the scattering image shown in Fig. 8(a). The difference between these two images is that they are complementary in terms of pixel intensity. That is because the solid parts of the phantom absorb more x-ray energy than hollow parts, which results in the dark parts in the absorption image, but meanwhile these solid parts create more scatter radiation, which ends up forming the bright parts in the scattering image. By comparing the photon number of the absorption

image (Fig. 9(b)) and the scattering image (Fig. 8(b)), it can be obtained that the photon detection efficiency of the proposed small-angle scattering detection system is roughly 1/3000 (one three-thousandth) when the phantom is 4 mm thick. Since it takes dozens of milliseconds to acquire a projection image during standard micro CT scanning with a resolution of dozens of micrometers, we can speculate that each exposure for our small-angle scattering detection system will need several seconds to dozens of seconds, which is acceptable in practice.

C. System Response Function

In this subsection, simulation tests were performed to study the response function and the angular resolution. Based on (17), we obtained the range of the principal angle and the angular resolution for a specific grating design. In the following, the first simulation was performed to demonstrate that these theoretical values agreed with the experiment results. Since the small-angle scattering intensity from one point was too small to be reliably detected, a parallel beam with a variable incident angle was used to simulate scattering signals. Two simulation tests with gaps of 280 μm and 120 μm were performed. The theoretical principal angles, the theoretical FWHM, and the measured FWHM are shown in Table 1. The detected signal profiles with respect to the variable incident angle are shown in Fig. 10. It can be seen that the peaks occurred respectively at 3.6° and 6.0°, which is consistent with the theoretical principal angles in Table 1. The corresponding measured FWHM values of the angular response curves are 2.8° and 4.18° which are close to the theoretical FWHM values in Table 1. These results suggest that the response function derived in Section II is correct. The principal angular range is $(0, w_1/h_1)$, according to (16), and it is $(0, 12^\circ)$ in this study. From Fig. 10, it can be seen that with the increment of the principal angle, the peak value of the response curve will decrease, which means that a smaller signal will be detected. Combining with the response equation (17) and the image formation equation (20), it is concluded that with the increment of the principal angle, the detected small-angle scattering signal will become more diffused, and the resolution will be lower. In other words, this method will produce a radiographic image of higher resolution with a smaller principal angle. Note that the proposed detection method integrates all the small-angle scattering photons instead of collecting the scattering signal along only one direction. Hence, our method will collect more energy and give a higher signal-to-noise ratio with a single exposure. At present, we can modify the principal angle and system geometric parameters to obtain a projective image at a good spatial resolution. A potential application is scatter tomography when we measure scattering projections from multiple directions. For small-angle scatter tomography, we would need to have the relationship between the small-angle scatter cross-section distribution and the detected projection data, which is analogous with the Radon transform [25] in traditional CT reconstruction. In Section II, we have derived the relationship in (20). In the following simulation, we can prove that (20) agrees with the simulation result which would lay a foundation for scatter tomography.

In the second simulation, a small cylinder phantom made of fat with a radius of 1 mm and height of 4 mm was put 2.2 cm away from the grating pair as illustrated in Fig. 11. Because the phantom is small, the attenuation of the scattering signal in the phantom can be ignored. In order to improve the signal-to-noise ratio, the total photon number was set to 2.0×10^{10} .

and the photon energy was set to 13 keV. For the sake of demonstrating that the proposed scheme can capture small-angle scattering signals from different angles by modifying the gap between the paired gratings, two numerical tests were performed with randomly selected gaps. The gap was 80 μm in the first simulation and 280 μm in the second simulation. According to (17), the corresponding principal angles are 7.2° and 3.6° . The small-angle scattering signals captured by our proposed scheme with different gaps are shown in Fig. 12(a). It is intuitive that the scattering signal from the cylinder phantom was of left-right and up-down symmetry. In fact, the detected image can be approximately regarded as circularly symmetric. If the designed cells have better isotropy, the scattering image will seem more circularly symmetric. The profiles along the central vertical lines of the images in Fig. 12(a) show two symmetric triangles (Fig. 12(b)). The peaks indicate the pixels that collected the most scattering signals. According to (17), we know that these peaks occur at the principal angle and we can calculate the locations of these peaks. The theoretical distance between peaks and the measured distance of the two simulations are shown in Table 2. It is evident that the theoretical distances and the measured distances are very close. From these results, we can conclude that the detected small-angle scattering signals are basically consistent with the response function derived in section II.

The average intensity of the two peaks in the blue profile is 1.5×10^{-7} , and the average intensity of the two peaks in the red profile is 1.26×10^{-7} . By subtracting the background scattering signal 0.596×10^{-7} from these two average intensity respectively, we can get the ratio of these two average intensity as 1.36. Since the radius of the phantom is only 5 pixels, we could assume that the scattering x-ray going out of the phantom will not be attenuated. On the basis of the response function in (17) and the image generation function in (20), we can numerically calculate the theoretical dotted profiles as shown in Fig. 13. The solid lines are the Monte Carlo simulation profiles shown in Fig. 12(b) subtracting background scattering. The theoretical profiles are similar to the Monte Carlo simulation profiles, and the ratio of peaks in the two profiles is 1.37 which is very close to the Monte Carlo simulation result. The errors are mostly due to quantum noise and a small portion of scattered x-rays passing through the boundaries of solid parts of the gratings. This result can validate that the derived response function is correct. Based on the result, we can also explain why the resolution of the scattering image decreases when the phantom is thicker in the resolution performance simulation. That is because when the phantom is thicker, more points in the phantom are far away from the grating, and the scattering signals coming from these points scatter more widely and cover a larger area which can blur the scattering image. Although a thick sample is a great challenge for our method at present, a validated response function will enable scatter tomography and address this issue in the future.

IV. DISCUSSION AND CONCLUSION

With theoretical analysis and Monte Carlo simulation, we have demonstrated that the proposed small-angle scattering detection scheme can collect small-angle scattering signals effectively and efficiently in parallel-beam geometry. In the simulation, the height of each grating cell was set to 120 μm to block all the primary x-ray photons of 20 keV. The principal incident angle depends on the values of height, width, and the gap of the grating

pair. Since the width and height of the grating are not easy to adjust in practice, the gap can be changed to determine the principal incident angle.

As far as image resolution is concerned, the thinner the phantom is, the higher the resolution of the detected small-angle scattering radiograph will be. That is why we can obtain a radiographic image with high resolution in the simulation. To give a theoretical formula to calculate resolution is not easy since the real resolution of the projective image is determined by multiple factors that are difficult to put in a simple closed-form formula. Nevertheless, we can use the distance between the symmetric peaks to estimate the resolution. At present, we have simulated the small-angle scattering radiography image of thin samples at high resolution, and validated the response function. Based on these results, we can build a new reconstruction model for tomography from small-angle scattering data. There are several dark-field forward models in the literature [21], [26] to address this problem. These existing methods will be helpful in our further study for small-angle scattering tomography with our proposed detection scheme. Eventually, small-angle scattering tensor tomography should be also very interesting [27].

For simplicity, we have performed this feasibility study in parallel-beam geometry. By limiting the range of the variable in (9) and (10) and/or bending the gratings and the detector surface, we can extend our scheme to fan-beam and cone-beam geometry. We expect that improving the isotropy of the response function will increase the image quality of the two-dimensional small-angle scattering image. Currently, the small-angle scattering image is of left-right and up-down symmetry. That is because the cell of the grating is squared. Hence, it is clear that if the cell is made hexagonal, it will improve the isotropy.

One limitation of x-ray small-angle scattering is that the amount of signals is less than one one-thousandth of the amount of attenuation signals. Hence, we are investigating how to improve the data acquisition efficiency. One way is to innovate geometry and characteristics of the gratings. Another way is to use a bright x-ray source, such as a Thomson scattering x-ray source, and more sensitive detectors, like photon-counting detectors.

Pathologically, small-angle scattering imaging can provide sensitive, specific, and unique information about soft tissues that x-ray attenuation images cannot show. Our proposed technology is new and effective to obtain a radiographic image practically. Also, we can develop tomographic techniques based on this detection scheme. We intend to prototype it as a novel tool for niche surgical and pathological applications.

In summary, we have proposed a new small-angle scattering imaging system featured by a pair of complementary x-ray gratings. This approach is focused on small-angle scattering signal detection, and should be practical when it is fully developed.

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Fig. 1.
Geometry of coherent scattering imaging.

Fig. 2.
Paired gratings for small-angle scattering imaging.

Fig. 3.
Geometrical parameters of the paired gratings.

Fig. 4.

One layer of the paired two-dimensional gratings from top view. The red units are the solid parts made of high-Z materials such as tungsten and gold, and the white units are the hollow parts. The second layer is complementary to this one.

Fig. 5.

The simulation for the validity of the EGSnrc software and the proposed detection scheme.

(a) Three different water phantoms with heights of 4 mm, 2 mm, and 1 mm were put respectively 0.6 mm, 1.6 mm, and 2.6 mm away from the grating. (b) The collected scattering images without (left) and with phantom (right). (c) The vertical profiles along the central lines of the two images in (b).

Fig. 6.

Polychromatic source and multi-material phantom simulation. (a) Three $2\text{mm} \times 2\text{mm} \times 4\text{mm}$ square cuboids made of three water, fat, and fibro-glandular are placed in front the grating; (b) The left is the small-angle scattering image from monochromatic x-ray, and the right is from polychromatic x-ray; (c) The vertical profiles along the central lines of the two images in (b); and (d) The vertical profiles along the central lines of the two images subtracting their respective backgrounds.

Fig. 7. Numerical phantoms used in performance simulation. (a) The first phantom with the radii from the innermost to outermost being 1 mm to 9 mm with common difference of 1 mm. (b) The second phantom contains only the outermost cylinder from the first phantom.

Fig. 8.

The detected scattering images from the phantom composed of concentric cylinders and their profiles. (a) The height of the phantom is 4 mm. (b) The vertical central profiles of the images in (a). (c) The height of phantom is 10 mm. (d) The vertical central profiles of the images in (c).

Fig. 9.

Detected absorption image in the simulation. (a) The absorption image of the same phantom as the one in Fig. 8(a). (b) The vertical central profile of the absorption image.

Fig. 10.

Angular response curves for two randomly selected cases in which the principal angle was set to 3.6° and 6° respectively.

Fig. 11. Small cylinder phantom with a height of 4 mm and a radius of 1 mm is put 2 cm away from the grating pair. (a) The sagittal view and (b) the coronal view.

Fig. 12.

Results from the phantom with a height of 4 mm, a radius of 1 mm, and placed 2 cm away from the grating. (a) The left is the detected small-angle scattering data when the principal angle is 7.2° ; the right one is when the principal angle is 3.6° . (b) The profiles along the central vertical lines of the two images in (a).

Fig. 13.
Comparison of theoretical profiles and Monte Carlo simulation profiles at different principal angles.

TABLE I

The comparison between the theoretical FWHM and the measured FWHM

Simulation	Principal angle	Theoretical FWHM	Measured FWHM
#1	3.6°	2.75°	2.8°
#2	6°	4.0°	4.18°

TABLE II

The comparison of the theoretical distance between peaks and the numerically simulated distance

Simulation	Principal angle	Theoretical distance between peaks (pixel)	Measured distance between peaks (pixel)
#1	7.2°	13.8	13
#2	3.6°	6.8	7