Local Orientation Dark-field Reconstruction

Masters Thesis in Computational Engineering

submitted
by
Shiyang Hu
born 16.08.1990 in Chengde, China

Written at
Lehrstuhl für Mustererkennung (Informatik 5)
Department Informatik
Friedrich-Alexander-Universität Erlangen-Nürnberg.

Advisor: Dr.-Ing. Andreas Maier, Prof. Dr.-Ing. Gisela Anton, Prof. Dr.-Ing. Joachim Hornegger
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Abstract

Dark-field signals are dependent on local orientations and are sensitive to small structural variations in objects. Grating-based X-ray dark-field imaging is a novel technique for gaining image contrast for object structures at size scales below setup resolution. Consequently, dark-field imaging produces images with superior contrast for weak absorption objects and reveals morphological information, leading it particularly beneficial for medical imaging and non-destructive testing. However, up to now algorithms for fully recovering the orientation dependence in a tomographic volume are still unexplored.

In this thesis, we propose a new reconstruction method for grating-based X-ray dark-field tomography. The presented algorithm is based on the formula in which an orientation-dependent signal is taken as an additional observable from a standard tomographic scan. The gradient descent method with zero constraints is the solution to the inverse problem. In detail, we extend the tomographic volume to a tensorial set of voxel data, containing the local orientation and contributions to dark-field scattering.

The presented algorithm is experimentally verified with a well-defined phantom, a fibrous wooden sample, a carbon fiber reinforced carbon (CFRC) sample, a dried peanut with an opening on its shell and a cotton fiber sample. In our experiments we present the first results of several test specimen exhibiting a heterogeneous composition in micro-structure, which demonstrates the diagnostic potential of the new method.
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Chapter 1

Introduction

1.1 Motivation

Conventional X-ray computed tomography (CT) has been widely used in clinics for therapy planning and treatment guidance since it is capable of providing various 3D anatomical structures by a non-invasive procedure. This technique yields excellent image contrast of objects for which high attenuation difference are obtained, e.g. between bones and soft tissues in human body.

However, for weak absorption objects, such as soft biological tissues or fiber composites, conventional X-ray imaging can not produce satisfactory results. To enhance the image contrast of this important object class, phase contrast and dark-field imaging have been investigated in the past years [Momose07, Jensen10].

Dark-field images describe X-ray small-angle scattering. A small-angle scattering signal is sensitive to granular and fibrous micro-structures with sizes in the range of the grating periods (e. g. 5 µm), which is remarkably smaller than the resolution of a medical imaging setup (e. g. 150 µm). As a result, dark-field imaging significantly enhances the image contrast for weak absorption objects and reveals morphological information of local orientations. As illustrated in Fig. 1.1 where absorption image, phase contrast and dark-field of cancerous mastectomy samples are presented, the dark-field image reveals the tumor area, which can not be observed in absorption image. This revolutionary and unique mechanism provides complementary and otherwise inaccessible information and has high potential in biomedical imaging, material science and other application fields [Pfeiffer08].

Periodic local orientation dependence can be observed from the dark-field signals. In Fig. 1.2 two series of dark-field images for a fiber bundle with elevation angle 15° (Fig. 1.2 (left)) and 60° (Fig. 1.2 (right)) are shown. From top to bottom, the six images are shown with changing
projection angles: $0^\circ, 18^\circ, 36^\circ, 54^\circ, 72^\circ$, and $90^\circ$. One observes that the dark-field signal varies periodically according to different projection angles. This angular dependence challenges traditional X-ray absorption imaging, attracting the attention to exploit the unique information which can be obtained from dark-field images.

Several approaches have been proposed in dark-field imaging. The theory of imaging with grating interferometer has been solidly founded [Haas10] [1]. A few dark-field tomography methods have been achieved in past years [Revol12, Malecki14]. However, no attempt has been made to fully reconstruct the 3D local orientations. Recently, Bayer et al. [Bayer13] presents the observation of periodic dark-field projections and illustrates the potential of exploiting full information of scanned objects. Hence, reconstruction methods for dark-field images based on the new local orientation-dependent dark-field scattering formula are needed. This will lead to new applications of dark-field images in medical diagnosis as well as non-destructive material science.

1.2 Previous Work

Research pertaining to local orientation dark-field imaging reconstruction includes fundamental physical theories, experiments and dark-field imaging reconstruction methods. The theory of dark-field scattering is well established, however, only few reconstruction algorithms have been
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Figure 1.2: Dark-field images of the fiber capillary for elevation angles 15° (left) and 60° (right). \( \phi \) denotes the rotation angle, in each column, six dark-field images at projection angles 0°, 18°, 36°, 54°, 72°, 90° have shown (from top to bottom). Minor Moiré patterns are visible in the images, images is reproduced under permission by [Bayer13].
CHAPTER 1. INTRODUCTION

formed specially for this frontier topic.

The mathematical concept for quantitative dark-field computer tomography (QDFCT) by linear diffusion coefficients was introduced by Bech et al. [Bech10]. They further demonstrated that a qualitative 3D reconstruction can be achieved when the dark-field scattering is isotropic.

Jesen et al. [Jensen10] illustrated that dark-field scattering depends on the orientation of the fibers with respect to the Talbot gratings and presented a simple scattering model to describe this angular dependence. The model is demonstrated by experiments of polypropylene fibers and a human tooth slice.

A very first exploration of the directional information with micro-structures in dark-field imaging of the specimen was obtained in the work of Potdevin et al. [Potdevin12]. The X-ray vector radiography (XVR) of human vertebra bone specimen was presented in their work and experimentally proves the feasibility of yielding structural information from XVR.

Yashiro et al. [Yashiro10] measured the coherent ultra-small-angle X-ray scattering of a penetrating X-ray wavefront in different samples and quantitatively formulated the reduction in visibility in X-ray Talbot interferometry. The formula is confirmed by the experimental results for microspheres and a melamine sponge.

Providing the angles of preferred orientations as prior knowledge, Revol et al. [Revol12] developed an orientation selective technique which allows for separating isotropic and anisotropic components of individual orientations. This reconstruction method was further verified by a wooden sample which contains two well-defined orientations.

Very recently, an attempt to reconstruct the local micro-morphology and its orientation in each voxel of the dark-field tomography was approached by Malecki et al. [Malecki14]. They formulated the product of directional scattering and the sensitivity vector of the directing interferometer based on a certain number of different scattering directions.

The reconstruction method in this thesis is based on the formulation from Bayer et al. [Bayer13]. In recently work, Bayer et al. observed the periodic dark-field projection and extended existing models of dark-field scattering to reveal angular dependence with respect to the local orientations by analyzing dark-field contrast (DFC) of carbon fiber reinforced carbon (CFRC). This novel model illustrated the potential of exploiting isotropic scattering information, anisotropic information as well as micro-structure information of a specimen. The empirical experiments presented in this thesis are in cooperations with Erlangen centre for astroparticle physics (ECAP) [http://www.ecap.physik.uni-erlangen.de/] and all dark-field projection data we are acquired in the ECAP.
1.3 Contributions of the Thesis

In this master thesis, angle-dependent dark-field tomography is investigated. A new reconstruction method for grating-based X-ray dark-field tomography is proposed and the method is further verified by a well-defined phantom as well as real data. Proper visualization illustrates the microstructures in tested specimens.

Research methodology followed in this master thesis includes the approach to recover the tensorial information in dark-field imaging and the empirical testing of the convergence of the algorithm and its feasibility to reconstruct real data.

1.4 Thesis Outline

The rest of this thesis is divided into 6 chapters. Chapter 2 presents the theoretical background of dark-field imaging and introduces the imaging procedure with Talbot-tau interferometer. In Chapter 3, a novel reconstruction method for dark-field scattering is proposed. Chapter 4 describes the experimental setup and materials has been used in this thesis. In Chapter 5 the reconstruction results are visualized and discussed. At last, Chapter 6 presents the potential future work and Chapter 7 concludes this thesis.
Chapter 2

Dark-field Imaging

2.1 Phase Contrast Imaging and Dark-field Imaging

Three different information sources can be measured from X-ray imaging: absorption, phase contrast and dark-field. The physical fundamentals are illustrated in Fig. 2.1. Symbols in the figure have the following meaning: $A_{REF}, I_0^{REF}$ and $\Phi_{REF}$ denote the amplitude, the offset and the phase of the reference X-ray wave, i.e. the X-ray wave without objects. $A_{OBJ}, I_0^{OBJ}$ and $\Phi_{OBJ}$ represent the amplitude, the offset and the phase of the objective X-ray wave with objects examined.

The total absorption along the X-ray beam is measured by the negative logarithmic ratio of the objective offset over the reference offset, i.e. $-\log(I_0^{OBJ}/I_0^{REF})$. An X-ray can be described as an electromagnetic wave, thus the phase of the wave will be shifted after the X-ray penetrates objects. The phase contrast measures the shift in phase $\Phi_{REF} - \Phi_{OBJ}$ (Fig. 2.1) of the electromagnetic wave passing through the objects. The imaging signal is essentially the first derivative of the wave-front phase profile along the transverse direction, which is perpendicular to the grating lines. The X-ray refraction results in sufficient phase shift for weakly absorbing materials, leading to significant enhancement of image contrast compared to traditional X-ray absorption imaging [Weitkamp06].

X-ray dark-field describes X-ray small-angle scattering, which is sensitive to structural variations and density fluctuation. Dark-field imaging measures the proportion of the interference visibility over the reference visibility $V_{REF}/V_{OBJ}$, where the visibility is given by the ratio of amplitude over offset, i.e. $V_{REF} = A_{REF}/I_0^{REF}, V_{OBJ} = A_{OBJ}/I_0^{OBJ}$ (see Fig. 2.1). The X-ray scattering offers remarkable contrast resolution of low attenuation classes of objects such as the soft biological tissues.
2.2 X-ray Imaging with Talbot-Lau Interferometers

Phase contrast imaging and dark-field imaging are both calculated from the wave profile. To obtain the wave profile, various X-ray based phase contrast and dark-field imaging techniques have been investigated in past years [Weitkamp06, Bech09, Yashiro10]. These techniques can be categorized into crystal interferometer, propagation based imaging, analyzer based imaging and grating based imaging. In the experiments of this thesis, we applied the one of grating based imaging specified as Talbot-Lau interferometers.

2.2.1 Fractional Talbot Effects

Talbot-Lau interferometers are based on the Talbot effect discovered in 1836 by Henry Fox Talbot. The Talbot effect is a near-field diffraction effect that shows periodic revival of a wavefunction after certain propagation distance, known as Talbot distance (Fig. 2.2), given by:

\[ z_T = \frac{2p^2}{\lambda}, \]  

(2.1)
2.2. X-RAY IMAGING WITH TALBOT-LAU INTERFEROMETERS

where \( p \) is the period of the wave, and \( \lambda \) is the wave length. From Fig. 2.2, it can be observed that at half Talbot distance, the wave-front appears with a transverse shift of half the grating period. At the fractional Talbot distances, the areas of highest and lowest intensity can be seen, which is referred to as the fractional Talbot effects.

2.2.2 Grating with Talbot-Lau Interferometers

The Talbot-Lau interferometers typically consists of the following parts: the X-ray source, the gratings G0, G1, G2 and the detector (Fig 2.3). Grating G0 is the source grating that splits the large source to smaller sub-sources. Grating G1 is the phase grating which splits the incoming beam into -1st and +1st diffraction orders, and generates an interference pattern at distance \( z_m = \frac{g_1^2}{8\lambda} \), \( g_1 \) is the period of G1. G2 is analyzer grating located at distance \( z_m \) from G1. G2 must have the same period as the periodicity of the fringe patterns caused by G1. If G1 has a phase shift of \( \pi \), then the periodicity of the fringe pattern is half the period of G1, i.e., \( g_2 = g_1/2 \). G2 consists of highly absorbing bars. The scanned objects have its own world coordinate system \( \hat{X}-\hat{Y}-\hat{Z} \) located in the world coordinate system \( \hat{x}-\hat{y}-\hat{z} \) (see in Fig. 2.3).

With Talbot-Lau interferometers, the experiments apply phase stepping to obtain phase contrast/dark-field scattering. In the phase stepping procedure, the analyzer grating G2 is shifted to plot the wave profile (Fig. 2.4).

As shown in Fig. 2.4, the image is recorded according to seven different transverse positions of the second grating G2. The image reaches lowest intensity at \( x_g = 0 \) and \( x_g = g_2 \) and highest intensity at \( x_g = g_2/2 \).

Phase contrast and dark-field images are extracted from the wave profile of each pixel obtained from the phase stepping procedure.

2.2.3 X-ray Dark-field Scattering Formula

The X-ray dark-field scattering formula is the foundation of the reconstruction algorithm. The formula is derived here following approach according to [Pfeiffer08, Jensen10, Bayer13].

The intensity \( I \) is given by:

\[
I = I_0 e^{-\int \mu(t) dt}
\]

(2.2)

where \( I_0 \) is the intensity of incident X-rays, known as offset in the wave profile in previous section and \( \mu(t) \) denotes the linear X-ray attenuation coefficient in the object along the traversed
Figure 2.2: Optical Talbot effect.
2.2. X-RAY IMAGING WITH TALBOT-LAU INTERFEROMETERS

Figure 2.3: The Talbot-Lau interferometers, image is provided by ECAP.

path \( t \). \( I \) can be reformed by first-order Fourier expansion,

\[
I(x_i, z_j, \omega) \approx a_0(x_i, z_j, \omega) + a_1(x_i, z_j, \omega) \cos \left( \frac{2\pi}{g_2} x_g - \Phi_1(x_i, z_j, \omega) \right)
\]  

(2.3)

where \( a_0, a_1 \) are the amplitude coefficient, \( \Phi_1 \) is the corresponding phase coefficient as shown in Fig. 2.5, \( g_2 \) is the period of grating G2 and \( x_g \) is the position along the transverse direction in which the gratings are scanned as shown in Fig. 2.4. And \( \omega \) is the rotation angle shown in Fig. 2.3.

As described in the previous section, the visibility contrast is given by:

\[
V(x_i, z_j, \omega) = \frac{V^\text{OBJ}(x_i, z_j, \omega)}{V^\text{REF}(x_i, z_j, \omega)}
\]

\[
= \frac{I^\text{OBJ}(x_i, z_j, \omega)}{I^\text{REF}(x_i, z_j, \omega)} \times \frac{A^\text{OBJ}(x_i, z_j, \omega)}{A^\text{REF}(x_i, z_j, \omega)}
\]

\[
= \frac{a_1^\text{OBJ}(x_i, z_j, \omega)}{a_0^\text{OBJ}(x_i, z_j, \omega)} \times \frac{a_1^\text{REF}(x_i, z_j, \omega)}{a_0^\text{REF}(x_i, z_j, \omega)}
\]

(2.4)

Scattering intensity from a single point can be modeled as a 2D Gaussian distribution. A 2D Gaussian distribution can be described as:

\[
f(x) = \frac{1}{2\pi \sqrt{|\Sigma|}} \exp \left( -\frac{1}{2} (x - \mu)^T \Sigma (x - \mu) \right)
\]

(2.5)

where \( x = (x^*, y^*) \), \( \mu \) is the mean matrix, \( \Sigma \) is variance matrix. In the dark-field scattering from
Figure 2.4: The phase stepping procedure, image is provided by ECAP.
a single point, we have:

\[ \mathbf{\mu} = [0, 0], \quad \mathbf{\Sigma} = \begin{bmatrix} \delta_1 & 0 \\ 0 & \delta_2 \end{bmatrix} \quad (2.6) \]

\( \delta_1, \delta_2 \) are width of the distribution in two axial directions. And the distribution is rotated by angle \( \psi_1 \), which is the local orientation of the pixel in \( X-Z \) plane, i.e.:

\[ \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} \cos \psi_1 & -\sin \psi_1 \\ \sin \psi_1 & \cos \psi_1 \end{bmatrix} \begin{bmatrix} x^* \\ y^* \end{bmatrix} \quad (2.7) \]

Thus, we have:

\[ S(x, y) = \frac{1}{2\pi \delta_1 \delta_2} \exp \left( -\frac{1}{2\delta_1^2}(\cos(\psi_1)x - \sin(\psi_1)y)^2 - \frac{1}{2\delta_2^2}(\sin(\psi_1)x + \cos(\psi_1)y)^2 \right) \]

\[ = \frac{1}{2\pi \delta_1 \delta_2} \exp\left(-\left(ax^2 + 2bxy + cy^2\right)\right), \]

\[ a := \frac{\cos(\psi_1)^2}{2\delta_1^2} + \frac{\sin(\psi_1)^2}{2\delta_2^2} \quad \] (2.8)

\[ b := \sin(\psi_1)\cos(\psi_2) \left(-\frac{1}{2\delta_1^2} + \frac{1}{2\delta_2^2}\right) \]

\[ c := \frac{\sin(\psi_1)^2}{2\delta_1^2} + \frac{\cos(\psi_1)^2}{2\delta_2^2} \]

As demonstrated in Fig. 2.6, the 2D Gaussian distribution \( S(x, y) \) has two axial directions, the first one is rotated by angle \( \psi_1 \). The scattering along the grating lines is negligible and the two gratings G1, G2 have the same direction, thus the dark-field signal can be calculated by
integrating $S(x, y)$ along $y$, resulting in:

$$S(x) = \int_{-\infty}^{\infty} S(x, y) dy$$

$$= \frac{1}{\sqrt{2\pi\delta^2}} \exp \left( \frac{-x^2}{2\delta^2} \right),$$

$$\delta = \frac{1}{2}(\delta_1^2 + \delta_2^2) + \frac{1}{2}(\delta_1^2 - \delta_2^2) \cos(2\psi_1 - \pi).$$ (2.9)

This formula of $S(x)$ is known as scattering function. The intensity after passing through the objects can be formed as the convolution of the reference intensity and the scattering function. Because that convolution in time domain equals the multiplication in Fourier domain, we have:

$$I^o(x) = I^r(x) * S(x)$$

$$= \hat{f}(\hat{f}(I^r(x))) \hat{f}(S(x)))$$

$$= a_0 + a_1 \exp \left( \frac{-2\pi^2\delta^2}{g_2^2} \right) \cos \left( \frac{2\pi}{g_2} x - \Phi_1 \right).$$ (2.10)
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tuting Eqn. 2.10 into 2.4, the following is obtained:

\[ V(\psi_1) = \exp\left(\frac{-\pi^2}{g_2^2}(\delta_1^2 + \delta_2^2)\right) \exp\left(\frac{-\pi^2}{g_2^2}(\delta_1^2 - \delta_2^2)\cos(2\psi_1 - \pi)\right) \]  

(2.11)

Noticing that in the Eqn. 2.11, \( \psi_1 \) is the relative angle of the objects at the point in X-Z plane regarding the experiment setup system. Therefore, when rotating with angle \( \omega \), the equation can be written as:

\[ V(\omega) = \exp\left(\frac{-\pi^2}{g_2^2}(\delta_1^2 + \delta_2^2)\right) \exp\left(\frac{-\pi^2}{g_2^2}(\delta_1^2 - \delta_2^2)\cos(2(\omega - \phi) - \pi)\right) \]  

(2.12)

where \( \phi \) is the angle of the objects according to its own coordinate system. Thus, the logarithm of the scatter dark field signal can be described as:

\[ D_s(\omega) = \log(V(\omega)) \]

\[ = -\frac{\pi^2}{g_2^2}(\delta_1^2 + \delta_2^2) - \frac{\pi^2}{g_2^2}(\delta_1^2 - \delta_2^2)\cos(2(\omega - \phi) - \pi) \]  

(2.13)

According to the double-angle formula:

\[ \cos(2A) = 1 - \sin^2(A) \]  

(2.14)

we have:

\[ D_s(\omega) = -\frac{\pi^2}{g_2^2}(\delta_1^2 + \delta_2^2) - \frac{\pi^2}{g_2^2}(\delta_1^2 - \delta_2^2)(1 - \sin^2((\phi - \omega) - \frac{\pi}{2})) \]

\[ = -\frac{\pi^2}{g_2^2}(\delta_1^2 + \delta_2^2) - \frac{\pi^2}{g_2^2}(\delta_1^2 - \delta_2^2) + \frac{\pi^2}{g_2^2}(\delta_1^2 - \delta_2^2)\sin^2((\phi - \omega) - \frac{\pi}{2}) \]

\[ = D_{iso} + D_{aniso}\sin^2((\phi - \omega) - \frac{\pi}{2}) \]  

(2.15)

where,

\[ D_{iso} = -\frac{\pi^2}{g_2^2}(\delta_1^2 + \delta_2^2) - \frac{\pi^2}{g_2^2}(\delta_1^2 - \delta_2^2) \]

\[ D_{aniso} = \frac{\pi^2}{g_2^2}(\delta_1^2 - \delta_2^2) \]  

(2.16)

\( D_{iso} \) is a measure of the isotropic scattering contribution, \( D_{aniso} \) is the amount of anisotropic scattering, which has maximum impact to the logarithmic dark-field signal at the angle \( \omega = \phi \).
CHAPTER 2. DARK-FIELD IMAGING

When the X-ray beam is penetrating though superposition of local orientated structures, the equation can be reformed as the sum of the contributions from different structures in the objects. Without losing generality, let us assume a ray penetrating the objects with \( L \) different structures, since only forward scattering at ultra-small angles contributes to the dark-field signal, the scattering of different structures in the first order is independent of other structures reacting with the ray. Assuming that scattering from the \( i \)th structure results in the Gaussian distribution of width \( \delta_i \), we have:

\[
\delta^2(\omega) = \sum_{i=1}^{L} \delta_i^2(\omega) \tag{2.17}
\]

which leads to the following visibility equation:

\[
D(\omega) = \sum_{i=1}^{L} d_{iso}(x, y, z) + d_{aniso}(x, y, z) \sin^2((\phi(x, y, z) - \omega) - \frac{\pi}{2}) \tag{2.18}
\]

where \( d_{iso}(x, y, z), d_{aniso}(x, y, z), \phi(x, y, z) \) denote the isotropic components, the anisotropic components and the angle at position \((x, y, z)\).

So far we discussed the dark-field scattering under the assumption that the entire beam are scattered. If parts of the beam is not scattered after passing through the objects, the visibility will be reduced and the equation should be modified according to the scattering portions. The assumption holds in this thesis because of the finite thickness and densities in the scanned specimens. Furthermore, as illustrated in following sections, the empirical testing results matched the presented model.

As illustrated in the function, dark-field scattering is dependent on the local orientation as well as the projection angle. Reconstruction of the dark-field scattering will reveal the morphological information of the structures in the specimens. In the work of Bayer et al. [Bayer13], dark-field signals of carbon fiber reinforced carbon (CFRC) and the fibers, both contains rich anisotropical structures, was analyzed. The projection data offer the possibility for a novel reconstruction method, which is suggested and evaluated in this thesis.
Chapter 3

Dark-field Reconstruction

3.1 X-ray Absorption Image Reconstruction

X-ray absorption imaging is an important diagnostic modality. The most commonly used method for reconstruction is the filtered backprojection, which is described in the following [Zeng10].

In a parallel beam imaging geometry, the projection can be described as:

\[ p(s, \theta) = \int_{-\infty}^{+\infty} f(x, y) \delta(x \cdot \theta - s) \, dx \, dy \]  

(3.1)

where \( x = (x, y) \), \( \theta = (\cos \theta, \sin \theta) \), \( \theta \) indicates the projection angle as demonstrated in Fig. 3.1, \( s \) is the distance of the straight line in the 2D object from the origin \((0, 0)\) and \( \delta \) is the Dirac delta function.

As shown in Fig. 3.2, the central slice theorem states that the 1D Fourier transform of the projection of a 2D function is equal to a line through the origin of the 2D Fourier transform of the function. This line is parallel to the projection sub-manifold. The central slice theorem can be expressed as:

\[ P(\omega, \theta) = F_{\text{polar}}(\omega, \theta), \]  

(3.2)

where \( P(\omega, \theta) \) is the 1D Fourier transform of \( p(s, \theta) \), given a certain \( \theta \), i.e.:

\[ P(\omega, \theta) = \int_{-\infty}^{\infty} p(s, \theta) e^{-2\pi i s \omega} \, ds \]  

(3.3)

\( F_{\text{polar}}(\omega, \theta) \) is the 2D Fourier transform of the intensity function \( f(x, y) \) in the polar coordinate.
system. The backprojected image $b(x, y)$ is calculated as:

$$b(x, y) = \int_{0}^{\pi} p(s, \theta) |_{s = x \cos \theta + y \sin \theta} d\theta \quad (3.4)$$

Based on the formulas above, we have:

$$f(x, y) = \int_{0}^{2\pi} \int_{0}^{\infty} F_{polar}(\omega, \theta) e^{2\pi i (x \cos \theta + y \sin \theta)} \omega d\omega d\theta$$

$$= \int_{0}^{2\pi} \int_{0}^{\infty} P(\omega, \theta) e^{2\pi i (x \cos \theta + y \sin \theta)} \omega d\omega d\theta \quad (3.5)$$

$$= \int_{0}^{\pi} \left( \int_{-\infty}^{\infty} P(\omega, \theta) |\omega| e^{2\pi i (x \cos \theta + y \sin \theta)} d\omega \right) d\theta$$

This can be reformulated to a two steps procedure:

$$q(s, \theta) = \int_{-\infty}^{\infty} P(\omega, \theta) |\omega| e^{2\pi i (x \cos \theta + y \sin \theta)} d\omega \quad (3.6)$$
Figure 3.2: Central slice theorem, image is reproduced under permission by Larry Zeng [Zeng10].
followed by:
\[
f(x, y) = \int_0^\pi q(s, \theta)|_{s=xcos\theta+y\sin\theta}d\theta \tag{3.7}\]

Eqn. [3.6] is filtering of the projections with the so-called ramp filter kernel $|\omega|$ and Eqn. [3.7] is the backprojection of the filtered projections. This procedure is known as filtered backprojection (FBP) reconstruction.

### 3.2 Dark-field Line Integral Model

Dark-field imaging allows to reconstruct micro-structures of a specimen on a length scale of few to few hundreds nanometers. The reconstruction results could reveal structures that have smaller sizes than the spatial resolution of the imaging system. The amount of scattering strongly depends on the structure orientations with respect to the X-ray scattering direction [Bayer13]. As shown in previous chapters, the physical model of X-ray dark-field imaging can be described by:

\[
d(x, y, z, \omega) = d_{iso}(x, y, z) + d_{aniso}(x, y, z) \sin^2 \left( (\phi(x, y, z) - \omega) - \frac{\pi}{2} \right) \tag{3.8}\]

where $\omega$ is the X-ray rotation angle and $\phi$ is the projected angle in X-Z plane at position $(x, y, z)$ (Fig. 2.3). $d_{iso}(x, y, z)$ and $d_{aniso}(x, y, z)$ are the isotropic and anisotropic components.

A parallel beam imaging geometry is applied in the experiments. As in such a system, reconstruction can be carried out within a plane with certain height $y$. Thus, for clarity, $y$ is omitted as follows:

\[
d(x, z, \omega) = d_{iso}(x, z) + d_{aniso}(x, z) \sin^2 \left( (\phi(x, z) - \omega) - \frac{\pi}{2} \right) \tag{3.9}\]

As discussed earlier in Eqn. [2.18] scattering from different structures in the projection line is independent from each other. Furthermore, experiments show that the amount of scattering decreases exponentially as the thickness of the specimen increases linearly. Thus, the line integral model of dark-field projection can be formed:

\[
P(s, \theta) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} e^{-d(x, z, \theta) \delta(x - s)} \, dx \, dz \tag{3.10}\]

where $x = (x, z), \theta = (\cos(\omega), \sin(\omega))$.

Let $D(s, \theta) = -\log(P/P_0)$ where $P_0$ is the reference signal measured with no objects exist.
The line integral model can be further discretized as ray sum:

\[
D(s, \omega) = \sum_{1 \leq i \leq M} \sum_{1 \leq j \leq N} d(x_i, z_j, \omega).
\] (3.11)

with the constraint that the positions \((x_i, z_j)\) of the contributing object voxels must lie on the line of sight of pixel \(s\) at rotation angle \(\omega\), i.e. \(x_i \cos(\omega) + z_j \sin(\omega) - s = 0\).

### 3.3 Inverse Problem

Orientation-dependent dark-field imaging reconstruction is the inverse problem of dark-field projection. Given the projection data and darkfield line integral model, the isotropic factor \(d_{\text{iso}}(x, y, z)\), the anisotropic factor \(d_{\text{aniso}}(x, y, z)\) and the structures showing by angles \(\phi(x, y, z)\) in coordinate system are desired. The filtered backprojection algorithm is discussed in previous section for reconstruction of X-ray absorption images. However, this reconstruction method is not applicable for dark-field imaging since the central slice theorem is not valid for dark-field imaging system due to the angular dependence. Other methods that can successfully reconstruct absorption images also can not be applied to dark-field reconstruction directly because of the same reason. Hereby, the inverse problem is tackled in the following approach:

According to the prosthaphaeresis formula:

\[
\cos(A + B) = \cos(A) \cos(B) - \sin(A) \sin(B)
\] (3.12)

and the periodic property:

\[
\sin(A + \pi) = -\sin(A), \quad \cos(B + \pi) = -\cos(B)
\] (3.13)

the discretized line-integral model could be derived as:

\[
d(x, z, \omega) = d_{\text{iso}}(x, z) - \frac{d_{\text{aniso}}(x, z)}{2} \cos(2\phi(x, z)) \cos(2\omega + \pi) - \frac{d_{\text{aniso}}(x, z)}{2} \sin(2\phi(x, z)) \sin(2\omega + \pi) + \frac{d_{\text{aniso}}(x, z)}{2}
\]

\[
= \begin{pmatrix}
    d_1(x, z) & d_2(x, z) & d_3(x, z)
\end{pmatrix}
\begin{pmatrix}
    1 \\
    \cos(2\omega) \\
    \sin(2\omega)
\end{pmatrix},
\] (3.14)
where

\[
\begin{align*}
    d_1(x, z) &= d_{iso}(x, z) + \frac{d_{aniso}(x, z)}{2} \\
    d_2(x, z) &= \frac{d_{aniso}(x, z)}{2} \cos(2\phi(x, z)) \\
    d_3(x, z) &= \frac{d_{aniso}(x, z)}{2} \sin(2\phi(x, z)).
\end{align*}
\] (3.15)

\[\forall s, \omega, \text{ Eqn. } 3.14 \text{ is linear combinations of three variables of each voxel lying in the line } x \cdot \omega - s = 0. \] The three variables are formed by the isotropic component, anisotropic component and the trigonometric functions of the local orientations. Thus, the inverse problem can be simplified as solving system of linear equations.

### 3.4 System Matrix Forming

Expanding Eqn. 3.11 by using Eqn. 3.14, we have:

\[
D(s, \omega) = \sum_{1 \leq i \leq M} \left( \begin{array}{c} d_1(x_i, z_j) \\ d_2(x_i, z_j) \\ d_3(x_i, z_j) \end{array} \right)^T \left( \begin{array}{c} 1 \\ \cos(2\omega) \\ \sin(2\omega) \end{array} \right)
\] (3.16)

Without loss of generality, we assume the object is discretized into \( M \times N \) image voxels. Let the detector length be \( S \), and the specimen is scanned from \( L \) different angles. The system of linear equations can be re-written in the matrix form as:

\[
D = MQd.
\] (3.17)

The exact content of \( D, M, Q \) and \( d \) is presented below. The overall goal is to estimate for each of the \( N \times M \) voxels in a reconstructed slice three unknown scatter coefficients in \( d \). \( d \) is reconstructed from the observations in \( D \) by selecting per detector cell the voxels that are traversed by a beam (using \( M \)) and transformed according to Eqn. 3.14 (using \( Q \)).

We proceed by defining the variables in Eqn. 3.4. Here, \( D \) is the logarithmic dark-field signal observed at the detector,

\[
D = [D(s_1, \omega_1), ..., D(s_G, \omega_L)]^T.
\] (3.18)

\( M \) is a \( SL \times LMN \) block matrix where \( m_{ij}^{st} \) is the contribution of voxel \((x_i, z_j)\) to the ray
3.4. SYSTEM MATRIX FORMING

\[ D(s,l), \]

\[ M = \begin{bmatrix}
  m_{11}^1 & m_{12}^1 & \cdots & m_{1N}^1 \\
  m_{11}^2 & m_{12}^2 & \cdots & m_{1N}^2 \\
  \vdots & \vdots & \ddots & \vdots \\
  m_{11}^L & m_{12}^L & \cdots & m_{1N}^L \\
  m_{S1}^1 & m_{S1}^2 & \cdots & m_{S1}^N \\
  \vdots & \vdots & \ddots & \vdots \\
  m_{SL}^1 & m_{SL}^2 & \cdots & m_{SL}^N
\end{bmatrix} \quad (3.19) \]

and \( Qd \) is the projected portion of the isotropic and anisotropic scattering, \( Q \) has the dimension \( LMN \times 3MN \), consisting of \( L \) sub-matrices for each angle \( \omega_i \):

\[ Q = \begin{bmatrix}
  1 \otimes \begin{bmatrix}
    1 & \cos(2\omega_1) & \sin(2\omega_1) \\
    \vdots & \vdots & \vdots \\
    1 & \cos(2\omega_i) & \sin(2\omega_i) \\
    \vdots & \vdots & \vdots \\
    1 & \cos(2\omega_L) & \sin(2\omega_L)
  \end{bmatrix} \\
  \vdots \\
  1 \otimes \begin{bmatrix}
    1 & \cos(2\omega_1) & \sin(2\omega_1) \\
    \vdots & \vdots & \vdots \\
    1 & \cos(2\omega_i) & \sin(2\omega_i) \\
    \vdots & \vdots & \vdots \\
    1 & \cos(2\omega_L) & \sin(2\omega_L)
  \end{bmatrix}
\end{bmatrix}, \quad (3.20) \]

where \( 1 \) is the \( MN \times MN \) identity matrix and \( \otimes \) denotes the Kronecker product. \( d \) is the unknown vector for which the system is solved. Let \( d_{k}^{i,j} = d_k(x_i, z_j) \) with \( 1 \leq k \leq 3, 1 \leq i \leq M, 1 \leq j \leq N \), then

\[ d = [d_{1}^{1,1}, d_{2}^{1,1}, d_{3}^{1,1}, \ldots, d_{1}^{M,N}, d_{2}^{M,N}, d_{3}^{M,N}]^{T}. \quad (3.21) \]

The non-ideal modeling of \( M \) generates deterministic errors between the projections \( D \) and the model \( MQd \), and further causes the noise in reconstruction. A more accurate re-sampling, given by bilinear interpolation, will reduce the deterministic errors.

Bilinear interpolation is an extension of linear interpolation (Fig.3.3). The value at point \( p = (x, y) \) is given by the linear combination of values at the nearest four grid points: \( Q_{11} = (x_1, y_1), Q_{12} = (x_1, y_2), Q_{1,3} = (x_2, y_1), Q_{1,4} = (x_2, y_2) \):

\[
  f(x, y) = \frac{1}{(x_2 - x_1)(y_2 - y_1)} \left( f(Q_{11})(x_2 - x)(y_2 - y) + 
  f(Q_{21})(x - x_1)(y_2 - y) + 
  f(Q_{12})(x_2 - x)(y - y_1) + 
  f(Q_{22})(x - x_1)(y - y_1) \right)
\]

\[ (3.22) \]
Using bilinear interpolation, the matrix $M$ is formed in following steps:

- generating the intersect points between $l$th projection ray and the object.
- calculating the coefficient of four nearest grid points bilinear interpolation formula $3.22$.
- calculating the sum of coefficients of image pixel at position $(x_i, z_j)$ associated with different intersect points (Fig. 3.4).

$$a_{ij} = \frac{x_1 y_{11}}{x_j y_1} + \frac{x_2 y_{12}}{x_j y_2} + \frac{x_{21} y_{22}}{x_j y_2}$$

Figure 3.3: Bilinear Interpolation

Figure 3.4: Element $m_{i,j}$
3.5 Prior Information Constrained Reconstruction

As stated above, an object can be reconstructed by solving a system of linear equations. However, in practice, it cannot be solved by direct methods due to the following reasons:

- Matrix $MQ$ is not square. Although generalized inverse can be used as the inverse of a non-squared matrix, it often cannot be obtained because of time and storage complexity.

- Even $MQ$ is square, its inverse will not exist if $MQ$ is not full rank.

- Noise usually causes inconsistencies of the projections.

- Often the matrix $MQ$ is too large to store, thus methods which require modifications on $MQ$ are not applicable.

The aforementioned limitations necessitates that $MQ$ is solved by iterative reconstruction methods. The advantages inherent to these methods are twofold: firstly they require only one row of $MQ$ be generated at each iteration; secondly, computational advances have improved them both in efficiency and efficacy.

3.5.1 Gradient Descent Algorithm

A standard approach for solving a system of linear equations is to compute the approximate solution of the least squares minimization problem. The solution of:

$$MQd = D$$

can be equally defined as minimizing the function:

$$f(d) = \|MQd - D\|^2$$

Gradient descent algorithm is a powerful iterative method for finding a local minimum of a function (Fig. 3.5). Starting from the initial point $x_0$, an iterative procedure can be formulated as:

$$d^{k+1} = d^k - t^k \nabla f(d^k),$$

where
CHAPTER 3. DARK-FIELD RECONSTRUCTION

\[ t^k: \] is the step length in the k-th iteration.

and where \( f(d^{k+1}) \) satisfies \( f(d^{k+1}) < f(d^k) \). Thus each iteration is further towards the minimum than the previous step. \( \nabla f(d^k) \) is calculated as:

\[
\nabla f(d^k) = \nabla((MQd - D)^T(MQd - P)) \\
= 2(MQ)^T(MQd - P)
\]

Gradient descent method is computationally effective and demands low storage. However, it has been theoretically proved that iterations for gradient descent method to converge is bigger than the condition number of a system matrix [Pyzara11]. The system matrix generated from image reconstruction problems is often ill-conditioned, thus the gradient descent method converges slow. Furthermore, the searching direction is not well-scaled, leading to the fact that number of iterations also depends on the scale of the problem [Box69]. Therefore, gradient descent method is less applicable in practical cases. Hereby, based on the traditional gradient descent algorithm, the gradient descent algorithm with zero constrains will be presented in the following section, in which prior knowledge is included.

3.5.2 Gradient Descent Method with Zero Constraints

In Chapter 2, we discussed the three type of information (absorption, phase contrast and dark-field) can be acquired in one experiment and conventional X-ray absorption imaging projections can be reconstructed by filtered backprojection. These reconstructed absorption images can be used as a supplement information in addition to the measurement of dark-field. A zero or negligibly small attenuation value indicates non-object regions which do not contribute to ultra-small-
angle scattering. Thus, we enforce the prior knowledge into the image by adding zero constrains to the optimization problem as described below.

As previously described, the inverse problem of dark-field images reconstruction is to solve a system of linear equations as follows:

$$MQd = D$$

Let $x_{abs}$ denote the reconstructed X-ray absorption image, from which we gain the prior knowledge on non absorption points. We define the active set that denotes the active zero points in nonnegative optimization problems by:

$$A(x_{abs}) = \{(i, j) \mid x_{abs}^{i,j} = 0\}$$

Further more, the active set of dark-field image can be deduced by

$$D(d) = \{(i, j) \mid (i, j) \in A(x)\}$$

Reforming system of linear equations as optimization problem, this prior information can be included as equality constrain, the problem becomes:

$$\begin{align*}
\text{minimize} & \quad \|MQd - D\| \\
\text{subject to} & \quad d_j = 0, j \in D(d)
\end{align*}$$

To reconstruct dark-field images slices equals to solve this constrained optimization. As described above, the unconstrained optimization problem can be solved by iterative gradient descent method, we embed the constraints by forcing the $d_j = 0$ where $j \in D(d)$ in each iteration. Consequently, this gradient descent with zero constrains is formulated as follows:

- **Step 1:** Initial $d^0 = 0$
- **Step 2:** $d^{k+1} = d^k + \lambda Q^T M^T (AQd^k - D)$, $\lambda$ is the searching step size set manually for different samples
- **Step 3:** Apply zero constraint to $d^{k+1}$, i.e set elements in $d^{k+1}$ to be zero according to the zero points in the reconstructed attenuation image
- **Step 4:** Repeat Step 2 and Step 3 until a convergence criterion is satisfied, in our case, the maximum of iteration numbers was used as the stopping criterion.
3.6 Visualization

Data visualization is essential for illustrating results which is concerned with quantitative analysis. In data visualization, information behind the data will be abstracted and expressed. Each voxel of dark-field image contains three dimensional information: structural information and their isotropic contributions as well as anisotropic contributions to the scattering. The method to reveal them visually is presented as follows.

3.6.1 Isotropic Field and Anisotropic Vector Field

For each voxel $\mathbf{d}_{i,j} = (d_{i,j}^1, d_{i,j}^2, d_{i,j}^3)^T$, the following equations are achieved:

\[
\begin{align*}
    d_1(x_i, z_j) &= d_{\text{iso}}(x_i, z_j) + \frac{d_{\text{aniso}}(x_i, z_j)}{2} \\
    d_2(x_i, z_j) &= \frac{d_{\text{aniso}}(x_i, z_j)}{2} \cos(2\phi(x_i, z_j)) \\
    d_3(x_i, z_j) &= \frac{d_{\text{aniso}}(x_i, z_j)}{2} \sin(2\phi(x_i, z_j)).
\end{align*}
\]

(3.25)

Solving this system of linear equations, we have:

\[
\begin{align*}
    d_{\text{iso}}(x_i, z_j) &= d_1(x_i, z_j) - \sqrt{d_1(x_i, z_j)^2 + d_2(x_i, z_j)^2} \\
    d_{\text{aniso}}(x_i, z_j) &= 2\sqrt{d_1(x_i, z_j)^2 + d_2(x_i, z_j)^2} \\
    \phi(x_i, z_j) &= \arctan \left( \frac{d_3(x_i, z_j)}{d_2(x_i, z_j)} \right).
\end{align*}
\]

(3.26) (3.27) (3.28)

Based on the parameters above, isotropic field and anisotropic vector field can be defined.

**Definition 1** (Vector field). A vector field is a continuous mapping:

$$
\mathbf{F} : U \subset \mathbb{R}^n \to \mathbb{R}^n,
$$

where $U$ is an open set on $\mathbb{R}^n$.

This definition can be interpreted as that a a vector field is an assignment of a vector to a point. For revealing the information in dark-field imaging reconstruction, the isotropic field and the anisotropic vector field are created as follow:
3.7 FRAMEWORK OF LOCAL ORIENTATION DARK-FIELD RECONSTRUCTION ALGORITHM

Definition 2 (Isotropic field).

\[ F_{\text{iso}}(d) = \{ d_{\text{iso}}(x_i, z_j) \mid i = 1, ..., M, j = 1 ... N \} \]

Definition 3 (Anisotropic vector field).

\[ F_{\text{aniso}}(d) = \{ (d_{\text{aniso}}(x_i, z_j) \cos(\phi(x_i, z_j)), d_{\text{aniso}}(x_i, z_j) \sin(\phi(x_i, z_j))) \mid i = 1, ..., M, j = 1 ... N \} \]

Isotropic field defines a projection assigned isotropic factor to its associate point. Anisotropic vector field defines a vector which expresses the direction scaled by the anisotropic factor to its associate point. To demonstrate the two fields visually, we applied an powerful open-source, multi-platform data analysis and visualization for vector field application-ParaView [www.paraview.org].

3.7 Framework of Local Orientation Dark-field Reconstruction Algorithm

The framework of local orientation dark-field reconstruction algorithm is shown in Fig 3.6.
Chapter 4

Experimental Setup

4.1 Investigated Samples

Four different samples were investigated in our tomography reconstruction study.

Wooden sample

A cubic wooden sample (see Fig. 4.1) was examined as first tomography specimen in our study. It consists of eight different layers, in each of which wood fibers are almost perfectly parallel aligned. The fiber orientations of consecutive layers are crossed at 90°, respectively, except of the second uppermost layer, which is rotated by 45°. The wooden sample has outer dimensions (L×W×H) of 11 mm × 9.5 mm × 9.5 mm. Each layer has a height of about 1.2 mm.

Figure 4.1: Wooden sample, image is provided by ECAP.
CHAPTER 4. EXPERIMENTAL SETUP

CFRC sample

The second investigated sample is an arrangement of blocks of carbon fiber reinforced carbon (CFRC). A sample block with dimensions of $44 \text{ mm} \times 6.0 \text{ mm} \times 5.5 \text{ mm}$ is shown in Fig. 4.2. The CFRC material blocks contain woven fabric sheets of carbon fiber bundles of some tenth of millimeter length, embedded in a quasi-amorphous graphite matrix that ensures the cohesion between the fibers and layers. The test sample consists of layers with cross-woven bundles forming a rectangular pattern. These layers are stacked to a bulk sample. The preferential directions of the fibers in different layers vary: the fibers in top and bottom layers are oriented along $x$- and $z$-axis (for $\omega = 0^\circ$). Two intermediate layers are rotated by $45^\circ$ around $y$-axis. One block (top left, cf. projection image in Fig. 4.2) is turned by $90^\circ$ around $x$-axis.

![Figure 4.2: CFRC sample, image is provided by ECAP.](image)

Peanut

The peanut (Fig. 4.3) was dried with one side opened. This sample forms an interesting biological specimen, exhibiting areas with predominantly isotropic or anisotropic scattering.

![Figure 4.3: Peanut sample, image is provided by ECAP.](image)
4.2. GRATING INTERFEROMETER SETUP

**Cotton fibers**

A cotton fibers sample was investigated at last. The cotton fibers sample contains two branch of carbon fibers with a diameter of 6 mm to 8 mm, one is positioned inside of a transparent glass pipe filled with cotton, the other one is placed outside of the pipe (Fig. 4.4). The outside one has the angle of 60° to z-axis (θ = 60°), and the inside fiber is orientated 15° to z-axis (θ = 15°). The projected angle into X-Z plane for both fibers are 0°.

![Figure 4.4: The cotton fiber sample, image is provided by ECAP.](image)

**4.2 Grating Interferometer Setup**

A polychromatic X-ray spectrum from a commercial rotating anode tube (MEGALIX CatPlus 125/40/90, Siemens AG, Germany) was used to illuminate the three gratings of the Talbot-Lau interferometer setup. The first grating downstream the X-ray tube is a source grating denoted as G0, assuring the horizontal spatial coherence as required for the subsequent configuration consisting of a phase grating G1 and an analyzer grating G2.

The heights of the grating bars are 8.7 μm nickel with period 4.37 μm for G1, and 150 μm and 110 μm gold for G0 and G2, respectively. The period of G0 is 23.95 μm, and 2.4 μm for G2. The distances are \( d_{G0-G1} = 161.2 \) cm and \( d_{G1-G2} = 15.9 \) cm. Radiographs are recorded downstream of G2 using a conventional flat-panel detector (Varian PaxScan 2520D, Varian Inc., USA) with CsI scintillator and a detector pixel sampling of 127 μm.

Differential phase-contrast and dark-field images are reconstructed from four phase steps of G2, each step being a regular fraction of \( p_2 \). Differential phase-contrast and dark-field values are
normalized to a bright-field reference with no sample in the beam, obtained by the same phase-stepping procedure [Weitkamp05]. Dark-field images are calculated from normalized visibility $V$ for every pixel of the detector matrix.

### 4.2.1 Image Acquisition

For the tomography scans, 601 (wooden and CFRC sample) or 361 projections (peanut) were taken over $360^\circ$, with four phase steps for each projection image. The X-ray tube was operated at 40 kV (wooden sample and peanut) or 60 kV voltage (CFRC sample) and a tube power of 2 kW. After every 25 projections, a reference image is taken to weaken image artifacts arising from thermic effects, detector properties etc. The experiment setup in ECAP lab can be seen in Fig. 4.5.
4.2. GRATING INTERFEROMETER SETUP

4.2.2 Technical Specifications

The technical specifications of hardware, software as well as programming languages to reconstruct the dark-field imaging presented in this thesis includes:

- **Programming languages:**
  - Java: Reconstruction algorithm in this thesis is programmed in Java.
  - Matlab: Matlab has been applied to plot the error measurements presented in following section.

- **Hardware:**
  - All implementations are accomplished on a computer based on Debian system with 4 cores Intel(R) Xeon(R) CPU/3.00GHz, 16-GB RAM and NVidia Corporation G86 [Quadro NVS 290] graphic card.

- **Software:**
  - Paraview: Reconstruction results are visualized in ParaView.
  - Inkscape: Images presented in this thesis are formated in Inkscape.
CHAPTER 4. EXPERIMENTAL SETUP
Chapter 5

Result and Discussion

5.1 Phantom

A prototype simulation phantom was created to examine the dark-field line integral model and evaluate the dark-field reconstruction algorithm with zero constrains. The phantom was a $20 \times 20$ pixel block positioned in an image of size $40 \times 40$ pixels. The block has the isotropic parameter $d_{\text{iso}}(x, z) \equiv 0.5$, the anisotropic parameter $d_{\text{aniso}}(x, z) \equiv 2$ and local orientation $\phi(x, z) \equiv 0$. The detector size is $60 \times 1$ and the pixel size is $1 \times 1$. The phantom was scanned from 361 projections over $2\pi$. This phantom was projected based on Eqn. 3.11. The projection sinogram is shown in Fig. 5.1 (a).

![Image](image.png)

Figure 5.1: Dark-field sinograms (a) of the prototype phantom, (b) of a horizontal slice of the fibrous wooden block.

Figure 5.2 shows the orientation-dependent dark-field values of the simulated digital phan-
tom as ground truth (column (a)) and its tomographic reconstruction (column (b)). The projection angles $\omega_i$ from top to bottom are $0^\circ$, $45^\circ$, $90^\circ$, $135^\circ$ and $180^\circ$. The image displays uniformly a minimum at projection angle $90^\circ$ and a maximum at projection angles $0^\circ$ and $180^\circ$. At projection angles $45^\circ$ and $135^\circ$, the image displays the values in between. Visually both ground truth (Fig. 5.2 (a)) and tensorial reconstruction (Fig. 5.2 (b)) match very well. This phantom is formed to simulate a single slice of the wooden sample presented in the following section. This phantom is designed to test the projection formula 3.11 and the convergence of the gradient descent algorithm with zero constraints. The projection formula will be verified by comparing the phantom sinogram with the sinogram of one slice of the wooden sample and discussed in next section, and the convergence of algorithm is examined below.

In order to quantitatively evaluate our method we calculated the errors separately for the isotropic component $d_{iso}(x, z)$, the vector magnitude $d_{aniso}(x, z)$ and the local orientation $\phi(x, z)$, and plotted them for each iteration in Fig. 5.3. The three different error measurement are all reduced to 50% of its initial value after three iterations and converges to zero in the end. This simulation phantom proves the convergence of the presented algorithm.

### 5.2 Wooden Sample

Fig. 5.1 (b) shows the sinogram of a horizontal slice of a tomographic measurement of a wooden block. Note the similarity with the phantom data in Fig. 5.1 (a), in particular the same periodic dark-field signal pattern. This similarity verifies the projection formula 3.11.

The orientation-dependent reconstruction of the wooden sample from 601 projections is presented in Fig. 5.4 by showing three representative layers: the 61st (Fig. 5.4 (a)), 99th (Fig. 5.4 (b)) and 141st layer (Fig. 5.4 (c)). The voxel size is $1 \times 1 \times 1$ and the detector has the dimension of $544 \times 250 \times 1$. For each layer, five images present the orientation-dependent dark-field $d(x, z, \omega_i)$ corresponding to five projection angles $\omega_i = 0^\circ$, $45^\circ$, $90^\circ$, $135^\circ$, and $180^\circ$. The orientation-dependency can be observed in each column. The phase of dark-field signal in layer (d) is shifted by $\frac{\pi}{4}$ from the phase in layer (c), and a phase shift of $\frac{\pi}{2}$ is obtained between layers (d) and (e).

In order to show that the reconstruction truly creates a model that matches the projection data, we investigated the raw data error [Zeng09] between the forward projection of our reconstruction and the captured raw data. The reduction in the raw data error is shown in Fig. 5.5. It is reduced to only 30% of the initial error after three iterations.

To illustrate the local orientation of the sample structure with its fibers with diameters in
Figure 5.2: Reconstructed slices illustrating the orientation-dependent dark-field values \( d(x, z, \omega_i) \). Each row voxel values with projection angle \( \omega_i = 0°, 45°, 90°, 135°, \) or \( 180° \) (from top to bottom), respectively. Columns (a) and (b) show ground truth and reconstruction result of the phantom. The arrows indicate the fiber orientation which could give maximum contribution to the dark-field measured for the given projection angle \( \omega_i \). If a region in the image is dark, it contains no fibers oriented in the arrow direction. Conversely, bright regions contain fibers oriented close to the arrow direction.
Figure 5.3: In the phantom simulation, the error in the isotropic and anisotropic contribution as well as in the angular component could be reduced to almost zero after less than 30 iterations.

The micrometer scale, the reconstruction result was visualized in Paraview [www.paraview.org]. The micro-structure denoted by $d_{\text{aniso}} \cos(\phi), d_{\text{aniso}} \sin(\phi)$ is visualized by lines. The length of the lines indicates the magnitude of the anisotropic contribution, $d_{\text{aniso}}$, to the scattering and the direction of the lines shows the structure orientation. Fig. 5.6 reveals different local orientations in different layers. The wooden sample was composed by 8 major plies. We chose the 45th, 61st, 81st, 99th, 130th, 141st, 151st, and 161st layer (from top to bottom) for visualizing the difference in structure orientation between the different plies. The second layer showed a $\pi/4$ orientation difference to the neighboring layers while all others were arranged at an additional rotation of $\pi/2$. This visualization is consistent with the reconstruction images shown above in Fig. 5.2 (c)-(e).

### 5.3 CFRC Sample

Four representative layers, the 37th, 63rd, 100th and 130th layer along the $y$-axis were chosen to demonstrate the orientation-dependent reconstruction of a CFRC sample, consisting of blocks aligned in different directions. These layers are shown column-wise in Fig. 5.7. In each row, from top to bottom, the presented projection angle is $\omega_i = 0^\circ, 45^\circ, 90^\circ, 135^\circ, 180^\circ$. In layer (c) and layer (d), which reflect the block shown in the photograph on top left of the figure, a periodic directional scattering pattern can be observed. Based on the tomographic reconstruction, the conclusion can be drawn that layer (d) has a periodic cross-woven structure that is aligned with the sample boundaries. The structure in layer (c) is rotated by $\pi/4$ compared to layer (d). The right block in layers (a) and (b) exhibited similar fiber orientations as the bigger, underlying block in (c) and (d). Hence, in layers (a) and (c), as well as layers (b) and (d), similarities in micro-structure could be observed for these areas. Generally, the sample structure of layers (a) and (b)
Figure 5.4: Reconstructed slices illustrating the orientation-dependent dark-field values $d(x, z, \omega_i)$. Each row voxel values with projection angle $\omega_i = 0^\circ, 45^\circ, 90^\circ, 135^\circ$, or $180^\circ$ (from top to bottom), respectively. Columns (a), (b), and (c) show representative reconstruction results of the wooden block in layers 61, 99 and 141, respectively (see photograph and dark-field projection image on top). The arrows indicate the fiber orientation which could give maximum contribution to the dark-field measured for the given projection angle $\omega_i$. If a region in the image is dark, it contains no fibers oriented in the arrow direction. Conversely, bright regions contain fibers oriented close to the arrow direction.
CHAPTER 5. RESULT AND DISCUSSION

Figure 5.5: The raw data error [Zeng09] for the wooden sample is reduced to 30% of its initial value after only three iterations (right).

Figure 5.6: Visualization of micro-structures of the 45th, 61st, 81st, 99th, 130th, 141st, 151st, and 161st layer of the wooden sample. The length of the lines indicates the magnitude of the anisotropic scattering contribution.
is complicated, as the contained fibers were both parallel and perpendicular to the rotation plane. As a result, only partly orientation scattering is reconstructed. More in detail, the left CFRC block in layer (a) shows the strongest scattering at $90^\circ$ on the lower half, while the right block showed the strongest scattering for its right corner at $45^\circ$, and for its left corner at $135^\circ$. In layer (b), both blocks exhibit the same pattern as the right block in layer (a).

The tomographic projection data for this experiment is considerably noisier than for the other experiments. Still, the raw data error also drops significantly (see Fig. 5.8). After 20 iterations, the error is reduced to 50% of its initial value. Note that the dimensions of the CFRC sample differ for the different orientations. The path length in the major axis is 44 mm while in the minor axis it is 6 mm.

Micro-structure was investigated by a visualization in Fig. 5.9. The slices (a) to (d) in Fig. 5.7 are displayed with their anisotropic component. Each line in these samples indicates the strength
and direction of the anisotropic portion (hence, a line in this visualization can run over the border of the object, if its anisotropic component is sufficiently strong). Varied in-plane directional information can be observed in this visualization. In both layers (a) and (b), the structure in the left block is roughly identical, while the right block exhibits a rotation of $\frac{\pi}{4}$ between layer (a) and (b). The main micro-structures in layer (c) are cross-woven, which forms a $\frac{\pi}{4}$ angle towards the sample boundary. Such cross-woven structures can be seen even better in layer (d). Here, bundles of lines all across the sample point into different directions. These findings are consistent with the true fiber orientation of the specimen, which can also be seen from the photograph of a sample block in Fig. 5.7 (top left).

5.4 Peanut Sample

In contrast to the wooden specimen and the CFRC sample presented earlier, a peanut shows less angular dependence (see Fig. 5.10). In each column from top to bottom, the imaging angle is again $\omega_i = 0^\circ, 45^\circ, 90^\circ, 135^\circ, 180^\circ$. From left to right, three representative slices are shown. We chose the 41st layer in which the tomography contains only peanut shell and the 100th and 133rd in which peanut shell, peanut seed coat and peanut cotyledon were present, respectively. Due to the fact that the peanut shell consists mostly of wooden fiber structure, the peanut shell part in each layer demonstrates the most directional scattering effect. Obviously, the waist of the peanut shell contains fibers in a direction which supports the mechanical stability of the shell. Nearly none angular dependent scattering can be observed from the cotyledon parts.

We furthermore investigated the raw data error over the iterations for the peanut sample. After 20 iterations, the error was reduced to about 15% of the original error as shown in Fig. 5.11.

To better illustrate the contributions of anisotropic scattering from different materials, we visualized the ratio of the anisotropic component over the isotropic component $d_{\text{aniso}}(x, z)/d_{\text{iso}}(x, z)$.
presented in Fig. 5.12. The magnitude in the visualization revealed the fact that the peanut shell had the highest anisotropy value among its three components. The seed coat parts, though very thin, differed in its ratio from the cotyledon. Most of cotyledon component had a ratio less than 1, which explains its weak orientation dependent behavior. The same materials in a different layer tended to keep the range of anisotropy ratio. Thus orientation-dependent dark-field reconstructions might be able to detect different materials through investigation of their anisotropic/isotropic ratio. In the tomographic images of cotton fibers sample, only the fiber brunch located outside the pipe demonstrates the orientation-dependent signal.

### 5.5 Cotton Fibers Sample

To illustrate the reconstruction of Cotton fiber sample, we chose a representative layer, the 270th layer along the \(y\)-axis. The projection angles \(\omega_i\) from left to right are \(0^\circ, 90^\circ, 180^\circ\). The fiber brunch positioned outside the pipe is shown as the lower part of the tomographic image in Fig. 5.13. Orientation-dependent signal can be observed from the outside fiber brunch while the fiber placed inside the cotton pipe (shown as the upper part in Fig. 5.13) demonstrated rarely changing of values. The dark-field imaging projections passing through the cotton pipe showed very few signal variations due to the strong isotropic property of the cotton (see in Fig. 5.14), leading to the unsuccessful reconstruction of the inside fiber. To distinguish anisotropic component from the strong isotropic component is thus desired in further work.

Further visualization of the projected angles into X-Z plane of the fibers can be seen from Fig. 5.15. The two fibers are positioned in the same azimuth angle, thus the results match the reality though the isotropic/anisotropic property can not be fully correctly reconstructed.
Figure 5.9: Visualization of micro-structures using the 37th (a), 63rd (b), 100th (c), and 130th slice (d) of the CFRC sample. The length of each line indicates the anisotropic scattering strength of a corresponding voxel and points in its predominant direction.
Figure 5.10: Dark-field projection image (top right) and tomographic reconstructions (bottom rows) of a peanut sample (see photograph on top left) in the 41st layer (a), 100th layer (b), and 133rd layer (c). Each column shows a series of dark-field scattering images with projection angles $\omega_i = 0^\circ, 45^\circ, 90^\circ, 135^\circ, 180^\circ$ (from top to bottom).

Figure 5.11: The raw data error for the CFRC sample is reduced to 50% after only three iterations.
Figure 5.12: Ratio of the anisotropic component over the isotropic component in 41st layer (top), 105th layer (middle), and 133rd layer (bottom) of the peanut sample.

Figure 5.13: Reconstructed slices illustrated orientation-dependent dark-field values \( d(x, z, \omega_i) \). Row voxel values with projection angle \( \omega_i = 0^\circ, 90^\circ, 180^\circ \) (left to right), the upper part presents the inside fiber brunch, the lower part presents the outside fiber brunch.

Figure 5.14: Dark-field sinogram of the 270th slice of the cotton fibers sample.
Figure 5.15: Visualization of the projected angles into X-Z plane of the two fiber brunch.
Chapter 6

Outlook

The separation of scattering contributions in dark-field reconstruction is a powerful concept. It enriches each voxel in the volume with the orientation and strength of the anisotropic scatter. Given the fact that this information can be recovered from a normal tomographic scan, it could become a standard source of information for medical diagnosis and investigation of non-detachable specimens in material testing. It is subject to future work to find out which tissue types or materials are best discriminated using directional dark-field information. However, one might speculate that potential benefits lie in the diagnosis of osteoporosis, where different bone structures have shown particular differences in the dark-field signa [Wen09]. Dark-field reconstruction might also be beneficial for the early detection of cancer. At a stage where malignant nodules are still very small, their signal in standard attenuation X-ray or MRI is weak. However, as the dark-field has the ability to visualize structural tissue variations below resolution limit of the system, the orientation-dependent dark-field reconstruction could have great impact on visualization of varying nodule vascularization, which is presented due to metabolic demands in tumor tissue already at early stages [Hillen07].

As the presented method is not generally limited by a small FOV, it can be used to investigate large specimen, assembly units, etc. Furthermore, the sensitivity to structures below imaging setup resolution is an essential advantage.

The projections of the investigated samples contain certain amount of noises [Weber11], which result in the difference between the projections calculated by the converged reconstruction and the experimental projections. No methods of filtering out the noises are applied in this thesis. Thus, reducing the noise from both the experiment setups and the improved algorithm with noise filters are needed in the future work.

Reconstruction of the cotton fiber sample illustrates that the solution of distinguishing anisotro-
opic objects from strong isotropic objects is still demanded. The well-reconstructed structure attracts the attention to explore the local orientations even without correctly reconstruct the isotropic and anisotropic components.

The algorithm is based on CPU programming and has the potential of speeding-up by applications of GPU-based programming. The presented algorithm can be interpreted in procedure of projection and backprojection, which are both highly parallel, thus the GPU-based programming is a very promising direction for further improvement.

The most appealing possibility lies in the fact that only in-plane angular dependence has been involved in the dark-field scattering function. A novel model of 3D angular dependence is thus desired and can lead to prominent outcomes.
Chapter 7

Summary

To overcome the unsatisfied image contrast for weak absorption objects such as biological soft tissues from conventional X-ray imaging, phase contrast and dark-field imaging have been investigated in recent years. Furthermore, grating-based X-ray dark-field imaging yields strong differences in the refractive index of a material at micrometer-scale, commonly subsumed as ultra-small angle scattering. Thus, dark-field imaging can reveal the morphological structures at the length below detector resolution, yielding the potential for novel diagnostic methods in medical imaging as well as approaches to non-destructive testing. In this work, a novel reconstruction for dark-field scattering was proposed. The presented reconstruction technique is based on the physical model of X-ray dark-field scattering, in which the local orientation dependence is described. This reconstruction method exploits the fully tensorial information of the scanned specimens.

Chapter 2 introduced the physical fundamentals for X-ray based imaging. Dark-field signals are measured by the proportion of the visibility of the object over the visibility of the reference, where visibility is given by the division of wave amplitude over the wave offset. The wave profile is obtained from phase stepping procedure by using Talbot-Lau interferometer. Dark-field scattering function can be deducted based on the following facts: firstly, scattering can be modeled as 2D Gaussian distribution, in which the scattering along grating lines will not contributed to the signal; secondly intensity after passing through objects can be formed as convolution of the reference intensity and the scattering function. The deducted formula illustrates the angular dependence of dark-field scattering. Furthermore, scattering from different structures in the projection line is independent from each other.

Chapter 3 is dedicated to the essential algorithm to reconstruct dark-field signals. We first introduced one of the most commonly used method, which is known as the filtered backprojection
method (FBP), to reconstruct X-ray absorption images. This FBP method is based on central slice theorem, which is not valid anymore for dark-field images due to the angular dependence. To overcome this problem, we presented the gradient descent method with zero constraints.

The underlying model formulates the X-ray dark-field signal as linear combinations of different directional scatterers in the beam path, hence being subject to a varying dark-field signal. For any ray, the projection is formed by line integral model, i.e. the summary of dark-field scatterings of the pixels that lies in the ray direction. The directional scatterers are formed by linear combinations of three coefficients composed of an isotropic component, an anisotropic component and a local geometric orientation. Based on this model the reconstruction problem can be formulated as a system of linear equations. In this system of linear equations, matrix of observed dark-field signals $D$ is given by the product of the matrix of unknown vectors $d$, the contributions matrix $M$ and the projected portion matrix $Q$. To reduce the deterministic errors, matrix $M$ is modeled by bilinear interpolation, in which value at a point is calculated by the linear combination of values at the nearest four grid points. As a solution to this system of linear equations, we proposed a gradient descent method with zero constraints in Chapter 3. The zero constraints are from FBP reconstruction of the X-ray absorption images obtained in the same experimental procedure. Non-objects regions are indicated by a zero or negligible small absorption value from the X-ray absorption images and such region will not contribute to dark-field scattering. In each iterative step of the gradient descent method, the zero constraints are applied by forcing the related values to zero. This method is possible to fully reconstruct for each voxel the isotropic component, the anisotropic component as well as the local orientation of the fibers in the specimen.

To illustrate the reconstruction results quantitatively, we presented a method to visualization dark-field reconstruction results by creating an isotropic field and an anisotropic field. The two fields are assignments of a dark-field scattering vector to a point that express the local orientations of each voxel and their contributions to dark-field scattering.

Three investigated samples were introduced in Chapter 4. The dimensions of the four tested samples were given and their structures were described. A fibrous wooden sample, which consists of eight different layers was presented firstly. The second examined sample was a CFRC sample, which consists of layers with cross-woven bundles forming a rectangular pattern. A common dried peanut with an opening on the shell was demonstrated. At last, a cotton fiber sample was shown. This sample contains a glass pipe filled with cotton, one branch carbon fibers positioned inside the pipe and the other branch of carbon fibers located outside of the pipe. The parameters of grating interferometer setup were presented later in that chapter, the model
of the polychromatic X-ray spectrum and the flat-panel detector as well as the dimensions of the grating bars were demonstrated, the image acquisition procedure were described. Software, hardware and programming language used in this thesis were introduced as technical specifications at last.

The presented algorithm was experimentally verified with the well-defined phantom, the fibrous wooden sample, the CFRC sample, the common peanut and the wooden fiber sample in Chapter 5. The similarity between the sinogram of a horizontal slice of a tomographic measurement of a wooden block and the phantom data verifies the projection formula. From the tomographic images of the wooden specimen and CFRC specimen, one can clearly observe the periodic directional scattering pattern as well as the shift of phase of dark-field signal in different layers. Furthermore, the tomographic reconstruction of the CFRC sample exhibits orientation-dependence, from which the cross-woven structure can be deduced. The peanut sample present the results of the algorithm when it is applied to mostly isotropic samples. Most directional scattering effect of the peanut sample is demonstrated by the waist of the peanut shell. The visualized ratio of the anisotropic component over the isotropic component in the peanut sample further illustrates that the peanut shell have the highest anisotropy in peanut.

Two different errors were measured. For the phantom, errors for the isotropic component, the vector magnitude and the local orientations are calculated separately. For wooden sample, CFRC sample, peanut sample as well as cotton fibers sample, the raw data error [Zeng09] are investigated. Error plot of each sample reveals the convergence of our algorithm.

The reconstruction results are visualized using ParaView. The micro-structures in examined specimens are visualized by lines and are denoted by \((d_{\text{aniso}} \cos(\phi), d_{\text{iso}} \cos(\phi))\). The anisotropic contribution to the scattering \(d_{\text{aniso}}\) is indicated by the length of the lines and the local orientation is shown by the line directions. The presented visualization results of wooden specimen and the CFRC sample illustrate the feasibility of retrieve morphological information of the investigated specimens both in-plane and in-layer. The CFRC specimen illustrates the potential of the algorithm for specimens which contains complex structures.

At last, Chapter 6 discusses the possible future implementations. Noise-reduced algorithm as well as GPU-base programming are desired. Dark-field scattering formula reveals the 3D angular dependence and reconstruction methods based on such a formula are appealing for further work.
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