A 3-D Projection Model for X-ray Dark-field Imaging

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ABSTRACT

Talbot-Lau X-ray phase-contrast imaging is a novel imaging modality. The setup uses gratings between a medical X-ray source and detector. It provides not only an X-ray absorption image, but also additionally a differential phase image and a dark-field image.

The dark-field image is related to small angle scattering from structures that range from hundreds of nanometers to a few micrometers. The dark-field signal has an interesting property when scanning oriented structures: the recorded signal depends on the relative orientation of the structure in the imaging system. Exactly this property allows to draw conclusions about the orientation and to reconstruct the structure, although the structure itself is much smaller than the resolution of the imaging system. However, the reconstruction is a complex, non-trivial challenge. A lot of research was conducted towards this goal in the last years and several reconstruction algorithms were proposed. A key step of the reconstruction algorithm is the inversion of a forward projection model. Up until now, only 2-D projection models are available, with effectively limit the scanning trajectory to a 2-D plane. To obtain true 3-D information, this limitation requires to combine several 2-D scans, which leads to quite complex, impractical acquisitions schemes. Furthermore, it is not possible with these models to use 3-D trajectories that might allow simpler protocols, like for example a helical trajectory.

To address these limitations, we propose in this work a very general 3-D projection model. Our projection model defines the dark-field signal dependent on an arbitrarily chosen ray and sensitivity direction. We derive the projection model under the assumption that the observed scatter distribution has a Gaussian shape.

We theoretically show the consistency of our model with more constrained existing 2-D models. Furthermore, we experimentally show the compatibility of our model with dark-field measurements of two matches. We believe that this 3-D projection model is an important step towards more flexible trajectories and, by extension, dark-field imaging protocols that are much better applicable in practice.

1 Introduction

The probably most studied acquisition system for X-ray phase-contrast imaging is the Talbot-Lau grating interferometer. This system allows to measure a X-ray absorption image and two additional images, namely the differential phase image and the dark-field image. The X-ray dark-field measures ultra-small-angle scattering, which is caused by inhomogeneities in materials at micrometer scale1–3.

Recently, X-ray dark-field imaging has received much attention for its potential applications in medical imaging and non-destructive material testing. The investigated applications in medical imaging span a wide range. Examples are the identification of different lung diseases4–7, lung cancer7, the identification of micro-calcifications9, or the differentiation of kidney stones10. Other examples are the detection of bone structures2 and fractures11 as well as brain connectivity12. Also for material testing there are a wide range of application of the dark-field signal3,13–16.

Two properties of the dark-field signal are particularly interesting. First, ultra-small angle scattering is caused by structural variations at the scale of few micrometers, which is significantly below the resolution of conventional X-ray imaging systems17. Second, a grating-based system allows to measure the 3-D orientation of elongated micrometer-sized structures such as fibers18,19. Traditional absorption X-ray systems have to be able to fully resolve a fiber in order to measure its orientation. In contrast to that, X-ray dark-field imaging enables to deduce the fiber orientation of considerably smaller structures.

The fundamental dependency of the dark-field signal between the orientations of the object and the imaging system has been explored by Jensen et al.20 and Revol et al.21. In a tomographic setup, either the object or the imaging system rotates during the acquisition. During the rotation, the relative orientation between object and system changes, which leads to a variation in
the signal. This signal variation allows to reconstruct the orientation of the structure. There have been several reconstruction methods proposed in previous works\textsuperscript{22–27}. However all of them are based on 2-D projection models of the 3-D structure. This means that the models rely on the reconstruction of several 2-D slices and are not compatible with true 3-D trajectories.

In this work, we aim to overcome this limitation by proposing a dark-field projection model over the 3-D space. This allows to directly estimate the 3-D structure, and to use sophisticated 3-D trajectories such as a helix.

1.1 Talbot-Lau Interferometer

The Talbot-Lau interferometer is a grating-based phase-contrast setup. A sketch of the system is shown in Fig. 1. The system is an extension from the conventional X-ray imaging setups, where three gratings $G_0$, $G_1$, and $G_2$ are placed between the source and detector. X-rays are generated by a conventional X-ray tube $S$. This X-ray tube can be operated in an X-ray regime that is compatible with medical applications. The X-rays are recorded by a medical X-ray detector $D$\textsuperscript{28, 29}. Grating $G_0$ effectively separates X-rays from the large source into narrow slit sources that are individually coherent, but mutually incoherent. $G_1$ imprints a periodic phase modulation onto the wave front to create an interference pattern at the detector. Both gratings $G_0$ and $G_1$ have periods that are in the range of few micrometers. To be compatible with the much lower resolution of clinical X-ray detectors, the interference pattern is sampled with the $G_2$-grating right in front of the detector, which also has a period in the range of micrometers. The sampling at the detector can be either performed by slightly detuning the grating $G_2$, which leads to the so-called Moiré effect\textsuperscript{30–32}, or by performing so-called phase stepping\textsuperscript{28, 29}. During phase-stepping, one of the gratings is moved laterally to sample different parts of the sinusoidal interference pattern while acquiring a stack of images. Both approaches, Moiré imaging and phase stepping, sample points on the interference curve, which can then be fitted by a sine. In practice, two scans are performed, a so-called reference scan without object in the beam path, and an object scan with the object. By comparing the sinusoidal curve of both scans, it is possible to calculate the three quantities absorption, differential phase, and dark-field. As in standard X-ray imaging, absorption is defined as the change in the average intensity. The differential phase is the angular shift of the sine. The dark-field signal is given by the ratio of the amplitude of the sine over the average intensity.

For this work, it is important to note that all three signal are created by sampling the sinusoidal function in one direction. We call this direction the sensitivity direction. The sensitivity direction is perpendicular to the grating bars.

1.2 Related Work

In a tomographic setup, either the object or the setup rotates during the acquisition. The rotation leads to changes in the relative orientation of the object with respect to the sensitivity direction, and therefore to a signal fluctuation of oriented structures.

This orientation-dependency of the dark-field signal introduces a notable difference to traditional X-ray computed tomography. The well-known filtered backprojection (FBP) algorithm is able to reconstruct the signal in a voxel by solving a linear system of equations. However, the use of FBP requires that the signal from a voxel is constant, and thus independent from the viewing direction. To this end, Schaff \textit{et al.}\textsuperscript{27} proposed to align the grating bars parallel to a 2-D trajectory. In this case, the sensitivity direction is perpendicular to the imaged plane, and the signal in each voxel is constant.

Other methods for orientation-dependent reconstruction align the grating bars perpendicular to a 2-D trajectory, such that the resulting signal per voxel varies along the trajectory. 2-D object orientations are in this case reconstructed via...
iterative reconstruction instead of FBP\textsuperscript{22–26}. Among these works, Bayer \textit{et al.} proposed a method to reconstruct 2-D in-plane orientations of fibers\textsuperscript{22}. Hu \textit{et al.} proposed to reconstruct the 3-D orientation by combining two 2-D in-plane scans with different trajectories\textsuperscript{23}. X-ray tensor tomography has been proposed by Malecki \textit{et al.}\textsuperscript{24}, Vogel \textit{et al.}\textsuperscript{25}, and Wieczorek \textit{et al.}\textsuperscript{26} by combining multiple 2-D planes.

All these reconstruction methods are designed to reconstruct 2-D projections of the object orientations from a 2-D trajectory. 3-D structural information is obtained in a second step by combining multiple 2-D reconstructions. The reconstruction of a structure (also in standard computed tomography) relies on the inversion of the projection model. Several projection models were proposed in 2-D for the angle-dependency of the dark-field. Jensen \textit{et al.}\textsuperscript{20} first showed the angle dependency of dark-field projections. They rotated the object around the optical axis of the system, and found that the variations in visibility can be described by the first two orders of the Fourier expansion. Shortly afterwards, Revol \textit{et al.}\textsuperscript{21} modeled the dark-field scatter by a 2-D Gaussian function and showed that the logarithm of the dark-field signal can be formulated as

\[
\hat{V}(\omega) = A + B \cdot \sin^2(\omega - \theta),
\]

where \(\omega\) is the rotation angle of the fiber around the optical axis, \(\theta\) is the starting angle of the fiber (see Fig. 2a) and \(A, B\) are an isotropic and anisotropic contribution of the scatter, respectively. The projection models\textsuperscript{20,21} assume that the object is rotated around the optical axis, which limits these models to thin sample layers. Malecki \textit{et al.}\textsuperscript{33} investigated the signal formation for the superposition of layers with different fiber orientations. They conclude that the dark-field signal can be represented as the line integral along the beam direction over the anisotropic scattering components. In order to describe the dark-field for 3-D data, Bayer \textit{et al.}\textsuperscript{17} proposed another projection model. They showed that the projection of a fibrous structure is also dependent on the azimuthal angle \(\phi\). This corresponds to the angle of the fiber projection in the x-z plane in Fig. 2b. They derive the dark-field signal as

\[
\hat{V}(\phi) = A + B \cdot \sin^2(\phi - \omega).
\]  

Recently, Schaff \textit{et al.}\textsuperscript{27} proposed to align the grating bars along the 2-D trajectory. Therefore, the dark-field signal is measured along the sensitivity direction along the y-axis. This leads to a constant signal, where the scattering strength depends on the angle between the fiber and the y-axis (see Fig. 2c).

However, all these projection models describe the dark-field only in 2-D, while the object creating the scatter is a 3-D structure. Previous works use several different ways to describe the 3-D nature of X-ray dark-field, ranging from Gaussian distributions\textsuperscript{20} over tensors\textsuperscript{25} to spherical harmonics\textsuperscript{26}. However, since all projection models describe the dark-field only dependent on one angle, the reconstruction the full 3-D distribution of oriented materials, requires the combination of scans from several trajectories, which overall leads to a quite complex acquisition protocols. Malecki \textit{et al.}\textsuperscript{24} reconstructed a scattering tensor by using the model from Revol \textit{et al.}\textsuperscript{21} and rotated the sample into a finite number of scattering directions. Hu \textit{et al.}\textsuperscript{23} used the model by Bayer \textit{et al.}\textsuperscript{17,22} and used two 2-D reconstructions to compute the 3-D fiber direction. Another example, is the very recent reconstruction model by Schaff \textit{et al.}\textsuperscript{27}. They fit a 3-D ellipse to individually reconstructed 2-D slices. In all cases the trajectory has a great impact on the numerical properties of the 3-D X-ray dark-field reconstruction. This becomes apparent when tomographic trajectories are chosen that operate only on a part of the full angular space around a sample. The probably most prominent example for such a situation is a helical trajectory. Here, the trajectory is continuously offset in out-of-plane direction.

1.3 Contributions and Organization of this Work

In this paper we propose a 3-D dark-field projection model. In contrast to previous works that describe the change of the dark-field for one 2-D trajectory, we propose a fully 3-D, direct description of the generated dark-field. This enables the use
of an arbitrary scanning geometry, and overcomes the need for combining several 2-D trajectories. Instead, established 3-D trajectories can directly be used, e.g., a helical geometry to acquire the 3-D scatter distribution, and novel 3-D geometries can be developed that explicitly aim at optimizing the recovery of directional information for clinical examinations or visual inspection tasks.

Additionally, the proposed model is very general. It allows to freely choose the ray direction and the sensitivity direction. That way, it overcomes the restriction of earlier works to parallel beam geometries, and allows to model a cone beam, which may be important, e.g., for a line scanner design.

We only use the assumption that the scatter distribution of the dark-field signal is a 3-D Gaussian, and we derive the general projection model from that. Furthermore, we discuss the impact of additional constraints if they are available, and demonstrate the consistency of the model with experimental dark-field measurements.

The paper is organized as follows. Section 2 provides a mathematical derivation of the proposed model, which describes the dark-field signal formation in a very general way. Afterwards, in Sec. 3, we discuss the impact of additional constraints on the model and show that our model is consistent with the 2-D projection models discussed in Sec. 1.2. Experiments that link the predicted signal to actual measurements are presented in Sec. 4. We conclude the paper in Sec. 5.

2 Proposed X-ray Dark-field Projection Model

The X-ray dark-field signal measures the X-ray small-angle scattering of microstructures in a sample. X-ray dark-field scattering has the special property that its observed magnitude can depend on the relative orientation of the sample in the setup. To characterize the signal from a sample point, we introduce the notion of isotropic and anisotropic scattering components. The scatter of the isotropic component is equally strongly observed, independent of the sample or setup orientation. Conversely, observations of scatter of the anisotropic component vary with the sample and setup orientation.

Thus, a purely isotropically scattering sample exhibits a constant signal per sample point, which can be similarly processed (e.g., in a reconstruction algorithm) as for example X-ray absorption. However, if a sample scatters (at least partially) anisotropically, the signal formation is considerably more complex. In particular, 2-D or 3-D reconstruction of the sample requires algorithms that explicitly take the direction-dependent signal variation into account.

In order to model the signal formation, we use the notion of a fiber as a microstructure that exhibits a mixture of isotropic and anisotropic scattering. We first expose the relationship between a fiber and its associated scatter distribution in Sec. 2.1. In Sec. 2.2, we show how the fiber is projected by the X-ray onto the sensitivity direction. The projected image of the fiber is then converted to a scatter distribution, which is the actually observed dark-field signature. This second step is described in Sec. 2.3. Afterwards, Sec. 2.5 shows how the measured signal can be expressed as line integrals.

The dark-field signal formation depends on three quantities, namely the directions of the X-ray and the dark-field sensitivity, and the orientation of the fiber. We describe a very general model that considers all three quantities as arbitrary vectors in 3-D. This generality has several advantages. It allows us to model not only a system with parallel beam and a perpendicular sensitivity direction, but instead arbitrary acquisition geometries. Examples for such more general system designs are the use of a cone-beam scanning geometry, which influences the ray direction, or the use of a curved X-ray detector, which results in different sensitivity directions. It also allows to model a 3-D helical scanning trajectory, which requires flexibility in all these quantities.

2.1 Relationship between Fiber and Scatter Distribution

We make the simplifying assumption that a fiber has the shape of a cylinder. More specifically, the fiber cross section is assumed to be a circle, and the rotation axis of the cylinder is assumed to be at least as long as the radius of that circle. The isotropic scattering component is mainly determined by the radius of the circle and will be more rigorously defined in Sec. 2.3.

Mathematically, we represent a fiber as a 3-D vector \( \mathbf{f} \) in \( \mathbb{R}^3 \), where the vector is parallel to the cylinder axis. The observed fiber creates dark-field scatter. Scatter is not deterministic, and therefore commonly described as a distribution.

For the following discussion, we are only interested in the relative orientations of the fiber and its associated scatter. Thus, without loss of generality, we assume that a fiber and its scatter distribution are rooted in the origin of the coordinate system.

We assume the scatter distribution of a fiber to be a 3-D Gaussian, which is compatible with earlier models on 2-D scatter distributions\(^{20}\). The main scattering direction of the fiber is the 2-D subspace that is perpendicular to \( \mathbf{f} \). This is illustrated in Fig. 3a.

The shape of the 3-D Gaussian function is completely described by its \( 3 \times 3 \) covariance matrix,

\[
g(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^3|\Sigma|}} \exp\left(-\frac{1}{2}(\mathbf{x}^\top \Sigma^{-1} \mathbf{x})\right),
\]

where \( \Sigma \) denotes the covariance matrix.
We make the mild assumption that this covariance matrix $\Sigma$ can be diagonalized (which is fulfilled for non-trivial Gaussian scatter observations). Then, the eigenvalues of $\Sigma$ describe the scatter strength with respect to its eigenbasis spanned by the eigenvectors $b_1, b_2, b_3$. The eigenvalues correspond to the variances, i.e., the squared standard deviations along each principal axis of the distribution:

$$\Sigma = \begin{pmatrix} \sigma_1^2 & 0 & 0 \\ 0 & \sigma_2^2 & 0 \\ 0 & 0 & \sigma_3^2 \end{pmatrix}. \quad (4)$$

These variances have a special distribution. Since the fiber primarily and homogeneously scatters in the directions perpendicular to the fiber direction $f$, the two largest eigenvalues $\sigma_1^2$ and $\sigma_2^2$ are identical, i.e., $\sigma_1^2 = \sigma_2^2$. The weakest scattering is observed in the direction of $f$, which is quantified by the smallest eigenvalue $\sigma_3^2 \leq \sigma_2^2$. This is illustrated in Fig. 3b. The eigenvector $b_3$, associated with the smallest eigenvalue $\sigma_3^2$, is parallel to $f$. More specifically, both vectors are identical with the exception that their sign might be flipped, i.e., $b_3 = \pm f$.

### 2.2 3-D Fiber Projection Model

The dark-field signal formation depends on three quantities, namely the directions of the X-ray and the dark-field sensitivity, and the orientation of the fiber. Ultimately, we seek the projection of the fiber along the ray direction onto the sensitivity direction. This is a mapping from the 3-D fiber vector onto a (1-D) scalar value. A non-parallel X-ray projection, e.g., from a cone beam, is modelled by a rotation of the fiber. The sensitivity direction can have an arbitrary orientation in space. To relate the fiber direction and the sensitivity direction, we introduce a virtual plane that is perpendicular to the X-ray. Both the fiber and the sensitivity direction are projected onto that plane. Then, the 2-D projection of the fiber onto the sensitivity direction in the plane is performed. The resulting equations show that the plane cancels, and that the projection of the fiber onto the sensitivity direction can directly be expressed with a scalar product. The mathematical derivation is presented below.

Let us consider a single fiber $f$. Without loss of generality, this fiber is located in the origin of our world coordinate system. The X-ray dark-field projection ray $r$ passes through that fiber, and thereby also the origin of the coordinate system. In imaging systems, all X-rays that form one projection are typically modelled as either parallel or diverging from an central ray $c$. This changes the relative orientation between $r$ and the fiber vector $f$. To correct for the diverging ray, we denote the angle of divergence as $\alpha$, and rotate the fiber in the plane spanned by $c$ and $r$ in the opposite direction. The corresponding rotation matrix is denoted as $R_\alpha$. In the case of parallel projection, $R_\alpha$ is the $3 \times 3$ identity matrix.

We project the fiber $f$ onto a plane that is perpendicular to the X-ray direction $r$. For this projection, we use orthogonal projections instead of perspective projections of the scatter pattern. This is possible, because the projection of a fiber signature
onto the detector is in the range of micrometers, but a single detector pixel is typically in the range of hundred of micrometers or more.

An orthogonal projection of a 3-D vector onto a plane can be performed with an inner product between the vector and a transformation matrix consisting of the 3-D coordinates of the 2-D basis. We define the 2-D projection plane as a plane where \( \mathbf{r} \) is the normal vector. Since \( \mathbf{r} \) passes through the origin, we find it convenient to choose the plane to also pass through the origin, i.e.,

\[
\mathbf{E} = (\mathbf{r}_{1}^{\text{ortho}}, \mathbf{r}_{2}^{\text{ortho}})
\]

with \( \mathbf{E} \in \mathbb{R}^{3 \times 2} \) where \( \mathbf{r}_{1}^{\text{ortho}} \) is a vector perpendicular to \( \mathbf{r} \), i.e., \( \mathbf{r} \mathbf{r}_{1}^{\text{ortho}} = 0 \), and \( \mathbf{r}_{2}^{\text{ortho}} = \mathbf{r} \times \mathbf{r}_{1}^{\text{ortho}} \) is the second vector spanning the plane, also perpendicular to \( \mathbf{r} \). This projection is visualized in Fig. 4 (left).

The projection of the fiber along the ray and onto the 2-D plane \( \mathbf{E} \) is then given as product of the rotated fiber \( \mathbf{f} \) with \( \mathbf{E} \), i.e.,

\[
\mathbf{f}' = (\mathbf{R}_{\alpha} \mathbf{f}) \mathbf{E}
\]

where \( \mathbf{f}' \in \mathbb{R}^{2} \) is now a two-dimensional vector in the plane \( \mathbf{E} \).

The sensitivity direction \( \mathbf{s} \) denotes the direction along which the X-ray dark-field signal can be measured. It is a 3-D vector with an arbitrary orientation. To relate the fiber with the sensitivity direction, we also project \( \mathbf{s} \) onto plane \( \mathbf{E} \). Analogously to the fiber-plane projection, we can also use here an orthographic projection. The 2-D projection of \( \mathbf{s} \) on \( \mathbf{E} \) is

\[
\mathbf{s}' = \mathbf{s} \mathbf{E}
\]

The projection of both vectors \( \mathbf{f}' \) and \( \mathbf{s}' \) on \( \mathbf{E} \) are shown in Fig. 4 (right).

To determine the alignment of the fiber \( \mathbf{f} \) with sensitivity direction \( \mathbf{s} \), the inner product is computed, i.e.

\[
\mathbf{f}'' = \mathbf{f}' \cdot \mathbf{s}'
\]

\[
= (\mathbf{R}_{\alpha} \mathbf{f}) \mathbf{E} \cdot (\mathbf{s} \mathbf{E}) = (\mathbf{E} \mathbf{R}_{\alpha} \mathbf{f}) \cdot (\mathbf{s} \mathbf{E})
\]

Equation 9 can be simplified by noting that the inner product commutes, which leads to

\[
\mathbf{f}'' = \mathbf{s} \cdot \mathbf{R}_{\alpha} \mathbf{f}
\]

since \( \mathbf{E} \mathbf{E}^\top = \mathbf{I} \). Equation 11 shows that the projection of the fiber through the system onto the sensitivity direction reduces to directly computing the inner product between the fiber and the sensitivity direction.

Note that in the case of a cone beam, the rotation of the fiber by \( \mathbf{R}_{\alpha} \) can also be replaced by a rotation of the sensitivity direction \( \mathbf{s} \) in the opposite direction. While we believe that the rotation of the fiber \( \mathbf{f} \) is more intuitive, it may be preferable for an actual implementation of a reconstruction algorithm to rotate the sensitivity direction \( \mathbf{s} \), since \( \mathbf{s} \) is a given quantity from the setup geometry, and \( \mathbf{f} \) is the unknown variable.

### 2.3 3-D Projection Model for Scattering

The projection of the fiber onto the sensitivity direction can be translated into the projection of the scatter. The scatter is the actually observed quantity in the imaging system. The inverse of this conversion links the observations to the unknown fiber direction.

The scatter distribution for a given fiber \( \mathbf{f} \) is given as

\[
\mathbf{f} \mapsto \begin{pmatrix} \sigma_{1}^{2} \\ \sigma_{2}^{2} \\ \sigma_{3}^{2} \end{pmatrix} \begin{pmatrix} \mathbf{b}_{1} \\ \mathbf{b}_{2} \\ \mathbf{b}_{3} \end{pmatrix}
\]

where \( \sigma_{i}^{2} = \sigma_{i}^{2} \), and \( \mathbf{b}_{1}, \mathbf{b}_{2}, \mathbf{b}_{3} \) are an orthogonal basis.

In Sec. 2.2 we considered the transformation from the 3-D fiber to a 1-D signal. We now want to describe this transformation for the scattering distribution. Since the distribution is described by an orthogonal basis, we can transform the basis vectors \( \mathbf{b}_{i} \) individually to get the transformation.

Since we defined our projection for an arbitrary fiber \( \mathbf{f} \), we can use the same mapping for each each basis vector \( \mathbf{b}_{i} \), i.e.,

\[
\sigma_{i}^{2} = \mathbf{s} \cdot \mathbf{R}_{\alpha} \left( \sigma_{i}^{2} \mathbf{b}_{i} \right)
\]
However, under the consideration that the scattering distribution is symmetric, the variance should not be dependent on direction of basis vector \( \pm b_i \). Rather we expect our observation to be of period \( \pi \). In analogy to previous 2-D models\(^{21, 22} \), this is addressed with the squared inner product. The projected variance is then

\[
\hat{\sigma}_i^{2n} = \left( s^\top \cdot R_{\alpha} \left( \sigma_i^2 b_i \right) \right)^2.
\] (14)

### 2.4 Complete 3-D Dark-Field Projection Model

With the individual projections of the fiber and the scattering distribution at hand, we combine both in this section to directly describe the scatter distribution for a given fiber. To this end, we use the introduced notions of isotropic and anisotropic scattering. The isotropic part results in an equal amount of scatter in all directions, while the anisotropic part depends on the relative orientation of the fiber, ray direction, and sensitivity direction. The goal is to describe the 1-D dark-field scattering signal in dependency of the fiber, since the fiber is the quantity we want to reconstruct in the end.

The observed dark-field signal is modelled as

\[
d = d_{\text{iso}} + d_{\text{aniso}} \left( s^\top \left( R_{\alpha} f \right) \right)^2.
\] (15)

Here, we again square the scaling factor of the anisotropic part to resemble the fact that the signal has a period of \( \pi \) instead of \( 2\pi \).

In 2-D models, the isotopic part is the amount that scatters in all directions equally, while the anisotropic part is an additional component in the direction perpendicular to the fiber direction. A schematic sketch of this model is shown in Fig. 5a. In 3-D, a direct adaptation of this approach is somewhat more complicated, since the additional scatter of the fiber perpendicular to its main axis forms a 2-D subspace. Instead, we find it more convenient to quantify the reduction of observed scatter in the direction of the main axis of the fiber, which is illustrated in Fig. 5b.

Thus, if we define the amount of isotropic and anisotropic scattering over the variances of the 3-D scattering function. The isotropic component is given as

\[
d_{\text{iso}} = \sigma_i^2 / 2,
\] (16)

while the anisotropic part is

\[
d_{\text{aniso}} = - \left( \sigma_i^2 - \sigma_3^2 \right).
\] (17)

To define the anisotropic part as the subtraction from the isotropic scattering may appear counter-intuitive at first glance. However, it allows to directly represent the fiber \( f \) in the model. We believe that it is useful for building a reconstruction algorithm on top of the model to have the fiber direction directly accessible, since it is the primary quantity of interest.

### 2.5 Dark-Field Line Integrals

In standard X-ray projection imaging, the measured signal intensity is the line integral along the X-ray beam line \( L \). Malecki \textit{et al.}\(^{33} \) showed that the superposition of dark-field signals is nothing else then a summation. The dark-field signal is then given by:

\[
D_L = \exp \left[ - \int_L d(x) \, dL \right].
\] (18)
3 Impact of Additional Constraints on the Model

The proposed projection model is very general. In this section we will show that it can be simplified under some assumptions and that it is consistent with the projection models by Revol\textsuperscript{21}, Bayer\textsuperscript{17}, and Schaff\textsuperscript{27}.

If we consider the model with a parallel beam geometry, then the Rotation matrix $R_{\alpha}$ is always the identity, i.e., $R_{\alpha} = \mathbb{1}$. Then, the anisotropic part of the dark-field only depends on the relative orientation of the fiber and sensitivity direction, thus

$$d = d_{\text{iso}} + d_{\text{aniso}} \left( s^\top f \right)^2. \quad (19)$$

We can now show that for these assumptions we are consistent with the 2-D projection models introduced in Sec. 1.2, if we consider a circular trajectory.

For the models by Revol\textsuperscript{21}, Bayer\textsuperscript{17} (Fig. 2a and Fig. 2b, respectively) the sensitivity direction lies in the trajectory plane, i.e., $s = (1, 0, 0)^\top$. Revol et al. rotates the fiber around the ray direction. Thus, the fiber orientation of $f$ in the x-y plane is dependent on the starting angle $\theta$ and the rotation angle $\omega$. We will denote this dependency as $f(\omega)$. The fiber is then given as

$$f(\omega) = \begin{pmatrix} \cos(\omega - \theta) & -\sin(\omega - \theta) & 0 \\ \sin(\omega - \theta) & \cos(\omega - \theta) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix} , \quad (20)$$

with $f = (f_x, f_y, f_z)^\top$. The dark-field model thus becomes $d = d_{\text{iso}} + d_{\text{aniso}} \left( (1, 0, 0)^\top f(\omega) \right)^2$, which can be transformed into the original formulation $A + B \cdot \sin^2(\omega - \theta)$. Similarly, the mapping to the model by Bayer et al. can be performed. Here the fiber is rotated around the y-axis. Then,

$$f(\omega) = \begin{pmatrix} \cos(\phi - \omega) & 0 & \sin(\phi - \omega) \\ 0 & 1 & 0 \\ -\sin(\phi - \omega) & 0 & \cos(\phi - \omega) \end{pmatrix} \begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix} , \quad (21)$$

which results to the original formulation $A + B \cdot \sin^2(\phi)$.

The model by Schaff\textsuperscript{27} (Fig. 2c) is based on the sensitivity direction perpendicular to the trajectory, i.e., $s = (0, 1, 0)^\top$. The dependency of the fiber is given a in Eq. 21. Then, the scaling factor of the anisotropic part is given as

$$f(\omega)' = (0, 1, 0) \begin{pmatrix} \cos(\omega) & 0 & \sin(\omega) \\ 0 & 1 & 0 \\ -\sin(\omega) & 0 & \cos(\omega) \end{pmatrix} \begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix} = f_y , \quad (22)$$

which is constant. Then the dark-field model is given as $V(\phi) = A + B \cdot c$, where $c$ denotes the constant anisotropic value.

In summary, the proposed model can be simplified to all three 2-D models that, to our knowledge, have been used in previous works. At the same time, however, the proposed model is general enough to also represent a full 3-D space where the directions of the X-ray, the fiber, and the sensitivity reside.

4 Experiments and Results

To evaluate the proposed projection model by comparing real and simulated dark-field signals. For that we use the scan of two matches. A detailed description of the Dataset can be found in Sec. 4.1. The experiment and results will be discussed in Sec. 4.2.

4.1 Dataset

In the following experiments, we analyze dark-field images of two matches. The two matches are glued to a block with a fixed relative position and angle (see Fig. 6a). The matchsticks have a thickness of $2.2 \pm 0.05$ mm, the head of the match about $3.2 \pm 0.1$ mm.

For the measurements, a Siemens MEGALIX CAT Plus 125/40/90-125GW medical X-ray tube with a tungsten anode is used. The data is acquired with an X-ray flat panel detector (PerkinElmer Dexela 1512) with 150 $\mu$m pixel pitch. The grating $G0$ has a period of 13.31 $\mu$m with a duty cycle of 0.5 and was positioned in a distance of 16.4 cm from the source. Grating $G1$ has a period of 5.71 $\mu$m. The duty cycle of $G1$ was 0.3, with 96.9 cm distance from the source. The grating $G2$ consists of a period of 10 $\mu$m, with a duty cycle of 0.5 and 157.4 cm distance from the source. The distance from the X-ray source to the sample is 81.8 cm and the distance from source to detector is 164.6 cm.

In each CT scan, 201 projection images over 360° are acquired with a 60 kVp spectrum using 1320 mAs per projection image. 16 phase-steps are performed for each projection image. After every 20th projection images, one reference image is
Figure 6. (a): Experimental setup. (b): Scanned object: two toothpicks. Dark-field images of two toothpicks at tilted angle: (c - e): $0^\circ$, (g - i): $30^\circ$, and (k - m): $-10^\circ$. (f, j, n): the intensity contrast of dark-field images in each column. Each column shows a series of three dark-field images obtained at the 1st, 26th and 79th rotation.
Averaged log dark-field measured simulated

Figure 7. Line plots of the Averaged log-dark-field signals of match samples titled at $-10^\circ$ from simulation (red) and experiment (blue).

taken. In total, five full tomographic scans are performed for different tilting angles of the sample. Figure 6 (c-m) shows three projection images from three scans. Each row shows the projections of different tilting angles of the matchsticks (0°, 30°, and $-10^\circ$, respectively), while each column shows different rotation angles, namely 0°, 44.8° and 139.7°.

4.2 Comparison of Simulated and Experimental Dark-field Signals
To analyse our proposed model, we show how well the calculated dark-field signals fit the respective experimental data. We use the data of the two matchsticks described in Sec. 4.1. Instead of using a true cone-beam geometry, our experimental setup provides an approximately parallel geometry. To simulate the dependency on the ray direction we tilt the angle of the matchsticks. We estimate the isotropic and anisotropic coefficient from the scans, with a tilted angle at 0° (Fig. 6c, 6d, and 6e) and 30° (Fig. 6g, 6h, and 6i). We use the negative logarithm of the obtained dark-field signals per detector pixel (so called log-dark-field) and average over a region of interest in each projection. The coefficients $d_{iso}$ and $d_{aniso}$ are fitted to the data from different tilt angles.

The proposed model is used to predict the dark-field signal for projections that were not used for fitting the data. In our experiment, we use the tilt angle at $-10^\circ$ for prediction, shown in Fig. 6k, 6l, and 6m. The normalized root mean square error (nRMSE) can be used to calculate the agreement to the measurements, which is given as

$$nRMSE = \frac{1}{d_{\text{max}} - d_{\text{min}}} \sqrt{\frac{\sum_{i=1}^{N_p} (\hat{d}_i - d_i)^2}{N_p}}$$ (23)

where $N_p$ is the number of projections, $d_i$ is the averaged log-dark-field at the $i$-th projection and $\hat{d}_i$ is the predicted value with our model at the $i$-th projection. $d_{\text{max}}$ and $d_{\text{min}}$ are the maximum and minimum value of the average log-dark-field value per projection of the measured data. In our experiments, the nRMSE is 5.3%.

A qualitative comparison is shown in Fig 7. The blue line depicts the averaged log-dark-field signal obtained from dark-field projections of matches at tilted angle $-10^\circ$. The red line shows the simulated values for the same dataset using the proposed projection model. The two wave forms show a high agreement. The main difference lies in a scaling factor of the data, which may come, e.g., from a somewhat too coarse estimation of the thickness of the matchsticks. Overall, the simulated results with our model and the real data-measurements fit very well together. This indicates that the model can be used for a full reconstruction of the data.

5 Conclusions and Outlook
In this paper, we propose an X-ray dark-field imaging projection model in which structural quantities are explicitly calculated in 3-D using the direction of the fiber, the ray direction and the sensitivity direction.

We believe that the new model is a potentially powerful tool for further development of X-ray dark-field imaging. In contrast to existing (2-D) projection models, where the imaging trajectory is explicitly (pre-)defined, our model allows to image arbitrary 3-D trajectories, such as a helix. We show that, while our model is more general than previous works, it is consistent with previous works if the additional constraints of these works are also applied to our model. Furthermore, we show that the model is consistent to real measurements by comparing predicted signals and experimental results from dark-field scans of two matches. In future work, we will use the proposed projection model to investigate the dark-field for true 3-D trajectories and to propose a reconstruction algorithm for such 3-D trajectories.
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