Magnified x-ray phase imaging using asymmetric Bragg reflection: Experiment and theory

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X-ray imaging using asymmetric Bragg reflection in the hard x-ray regime opens the way to improve the spatial resolution limit below 1 µm by magnifying the image before detection, simultaneously providing a strong phase contrast. A theoretical formalism of the imaging process is established. Based on this algorithm, numerical simulations are performed and demonstrate that both Fresnel propagation and Bragg diffraction contribute to contrast formation. The achievable resolution of this technique is investigated theoretically; the results obtained can be used to improve future experimental setups. Furthermore, the minimum detectable phase gradient is estimated, for comparison with other phase sensitive imaging techniques. Results from biological objects demonstrate that the technique is viable for imaging both in two and three dimensions. Refraction contrast images are extracted from experimental projection images by an algorithm similar to diffraction-enhanced imaging (DEI), and used to achieve three-dimensional tomographic reconstruction.

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I. INTRODUCTION

Contrast enhancement in x-ray imaging can be achieved by exploiting phase contrast in addition to absorption contrast. This is particularly advantageous in the case of light organic, weakly absorbing objects. One of the most often used techniques for experimentally obtaining phase contrast is Fresnel propagation or in-line holography.1–4 A principal alternative is analyzer-based imaging, also known as diffraction-enhanced imaging (DEI).5

DEI is based on the combination of transmission of an x-ray wave field through the object under study (radiography) with subsequent Bragg diffraction at an analyzer crystal. Owing to the narrow angular range of Bragg diffraction, the analyzer efficiently selects rays locally deviated at the object by specific angular amounts due to phase gradients within the sample, thus enhancing image contrast.

This technique has proven useful for the investigation of laser-fusion targets,6 for x-ray diffraction topography,7 and biological and medical imaging.8 Advanced analysis techniques have been developed5,8–10 which combine several images taken at different angular positions of the analyzer crystal. In this way, the effects of x-ray absorption, refraction, and small-angle scattering can be experimentally separated and a set of complementary images with specific contrast features is obtained.

While the standard DEI setup is based on symmetric reflection from the analyzer surface, asymmetric reflections make it possible to simultaneously realize image magnification.8 By using two consecutive reflections from a pair of analyzers, magnification can be achieved in both image dimensions.7,9,11–13 For a given analyzer surface orientation, the magnification factor uniquely depends on the x-ray photon energy. Synchrotron radiation is advantageous, since its energy tunability gives one the flexibility to widely vary the magnification by small changes in energy.

Asymmetric-reflection DEI thus opens the way to phase-contrast imaging with sub-micrometer spatial resolution. It represents a path out of a conflict encountered in direct x-ray imaging: Particularly when using state-of-the-art CCD cameras, spatial resolution improvements usually require reducing the converter screen thickness, at the expense of detection efficiency. By exploiting post-transmission image magnification, commercial CCD cameras with moderate pixel sizes but high sensitivity remain usable even for applications requiring highest spatial resolution.

In this way, magnified x-ray imaging allows one to simultaneously realize submicrometer resolution and phase contrast. While the magnification factor is seemingly unlimited, the actual resolution is determined by a complex interplay of several concurring factors. For a precise determination of resolution limits, a complete theory of the imaging process is therefore mandatory; resolution cannot simply be equated with geometrical quantities such as the projected x-ray penetration depth in the analyzer.

In this article, we present an instrumental realization of the principle of magnified imaging—the “Bragg Magnifier”—optimized in view of high spatial resolution. In the theoretical part, a comprehensive description of the image formation process is developed, including wave propagation behind the object (Fresnel diffraction) and reflection at the analyzer crystals (Bragg diffraction). Based on this theory, the achievable spatial resolution is estimated numerically for several different scenarios and model objects. The results reveal significant differences between the limiting cases of absorption objects and phase objects. Moreover, implications for further instrumental optimization are deduced. The phase sensitivity of the technique is quantified. An example of an experimental measurement performed on biological objects will be shown, including results of three-dimensional imaging after tomographic reconstruction.

II. THEORY OF IMAGE FORMATION

In this section we will discuss the image formation of the Bragg magnifier sketched in Fig. 1: A monochromatic wave is transmitted through the sample and diffracted twice by two
are neglected here, as commonly done in the literature.

B. Fresnel approximation

Applying three-dimensional Fourier transform to the three wave fields \( D_i(r_i) \) leads to their Fourier presentations \( \tilde{D}_i(k_i) \):

\[
D_i(r_i) = \int d^3k_i \tilde{D}_i(k_i)e^{i k_i \cdot r_i}.
\]

We will now demonstrate that in case of monochromatic waves Fresnel propagation (i.e., free-space propagation of the x-ray beam after transmission through the sample) is already described by Eq. (2). A similar discussion in Fourier space leading to the same result can be found in Ref. 14.

The monochromaticity restricts the possible wave vectors \( k_i \) to those fulfilling \( |k_i| = \frac{\omega}{c} \) with \( \omega \) the angular frequency and \( c \) the vacuum speed of light, and therefore the corresponding three-dimensional wave field is only nonzero on the surface of a sphere with radius \( |k_i| \). Expressing the wave vector \( k_i \) by deviations \( q_i \) from a reference vector \( k_0i \), the latter pointing in main beam direction, written in components

\[
k_i = k_0i + q_1i e_{1i} + q_2i e_{2i} + q_3i e_{3i}
\]

(3)

the small angle approximation \( q_i \ll |k_i| \)—this is Fresnel approximation in Fourier space—can be performed by concluding

\[
k_i^2 = k_0i^2 + q_1i^2 + q_2i^2 + q_3i^2 + 2k_0iq_i \Rightarrow q_i = -\frac{1}{2k_i}(q_1^2 + q_2^2).
\]

(4)

Due to the monochromaticity, the argument of the integral (2) can be multiplied by a Dirac delta function \( \delta_{|k|-\frac{|k|}{c}} \) and the corresponding sphere can be replaced by a rotation parabola at \( k_0i \), yielding

\[
D_i(r_i) = \int dq_1dq_2\hat{D}_i(q_1, q_2)\delta(q_1^2 + q_2^2 - (2k_iq_1^2 + 2k_iq_2^2)),
\]

(5)

where \( \hat{D}_i(q_1, q_2) \) is the two-dimensional Fourier representation of the amplitude in the \( xy \) plane at \( z_i = 0 \). Equation (5) is exactly the Fresnel integral in Fourier space.

C. Diffraction integral of the Bragg magnifier

The dynamical theory of diffraction connects a single wave before the reflection to a single wave after the reflection, where the wave vectors are related by

\[
k_i = k_{z_{i-1}} + g_i + \Delta_i(k_{z_{i-1}})\hat{n}_i \quad (i = 1, 2).
\]

(6)

\( g_i \) is the reciprocal lattice vector of the reflection \( i \), \( \Delta_i(k_{z_{i-1}}) \) is the deviation parameter and \( \hat{n}_i \) are the normals of the analyzer surfaces. The wave amplitudes themselves relate in the following way:

\[
\hat{D}_i(k_i) = \hat{D}_{z_{i-1}}(k_{z_{i-1}})\hat{R}_i(k_{z_{i-1}})e^{-i\Delta_i(k_{z_{i-1}})\hat{n}_i r_{i0}} \quad (i = 1, 2),
\]

(7)

where \( \hat{R}_i \) is the reflectivity of the \( i \)th reflection, which can be calculated from dynamical theory of x-ray diffraction.\(^{15}\)
Standard dynamical diffraction theory is valid for a coordinate system with its origin on the surface of the crystal and therefore the additional phase factor $e^{-i\Delta(k_{\mathbf{r}})\mathbf{r}_0}$ in Eq. (7) takes an arbitrary origin $\mathbf{r}_0$ into account. If $\mathbf{d}_1$ is the vector linking the sample origin and the first analyzer surface and $\mathbf{d}_2$ is the vector linking the first analyzer surface with the second, then $\mathbf{r}_0=\mathbf{d}_1$ and $\mathbf{r}_0=\mathbf{d}_1+\mathbf{d}_2$ are valid. Using the above equations and with $\mathbf{r}_2=\mathbf{r}-\mathbf{d}_1-\mathbf{d}_2$ it is easy to show that

$$D_2(\mathbf{r}_2) = \int d^3k_2 \hat{D}_0(\mathbf{k}_0) \hat{R}_1(\mathbf{k}_0) \hat{R}_2(\mathbf{k}_1) e^{i(k_2 \mathbf{r}_2 + k_1 \mathbf{d}_1 + k_0 \mathbf{d}_1)}$$

(8)

is valid.

Using substitution we will rewrite Eq. (8) to components of the original coordinate system ($q_{x0}$, $q_{y0}$, and $q_{z0}$), i.e., the coordinate system for the wave field before any reflection. For this purpose we will first connect the wave vectors before and after the first reflection. The reference wave vectors $\mathbf{k}_{00}$ and $\mathbf{k}_{01}$ defined in the same way as the reference vector in Eq. (3) are connected by $\mathbf{k}_{01} = \mathbf{k}_{00} + \Delta q_1 \hat{n}_1$ with $\Delta q_1 = \Delta q(\mathbf{k}_{00})$. Using the components of $\mathbf{k}_1$ and $\mathbf{k}_0$ similar to Eq. (3) and Eq. (6) leads to

$$q_{x1} e_{x1} + q_{y1} e_{y1} + q_{z1} e_{z1} = q_{x0} e_{x0} + q_{y0} e_{y0} + q_{z0} e_{z0} + (\Delta q_1 - \Delta q_0) \hat{n}_1.$$  

(9)

By multiplying with the vector $\hat{n}_{1z}$, which is perpendicular to $\hat{n}_1$ and lies in the $xz$ plane we get

$$q_{x1} e_{x1} + q_{y1} e_{y1} + q_{z1} e_{z1} = q_{x0} e_{x0} + q_{y0} e_{y0} + q_{z0} e_{z0} + \Delta q_1 \frac{\mathbf{e}_{z0}}{\mathbf{\hat{n}}_{1z}}$$

(10)

The use of the Fresnel approximation, implying $q_{x1} \approx q_{y1}$, justifies the first order approximation $q_{x1} = -\frac{1}{m_1} q_{x0}$, where $m_1$ is the magnification factor of the first reflection. Consequently, $q_{z1} = -\frac{1}{2k} \left( \frac{1}{m_1^2} q_{x0}^2 + q_{y0}^2 \right)$ holds [Eq. (4)]. By inserting this into Eq. (10) the second order approximation

$$q_{x1} \approx -\frac{1}{m_1} q_{x0} - \mathbf{m}_1 q_{x0} + \mathbf{m}_1 \frac{1}{2k} \left( \frac{1}{m_1^2} q_{x0}^2 + q_{y0}^2 \right)$$

(11)

is obtained. With similar reasoning there is further the trivial result

$$q_{y1} = q_{y0}$$

(12)

which was already used in Eq. (11). Presuming that the two magnification directions are perpendicular to each other (i.e., avoiding shear effects) an analogous discussion for the second reflection leads to

$$q_{y2} \approx -\frac{1}{m_2} q_{y0} - \mathbf{m}_2 q_{y0} + \mathbf{m}_2 \frac{1}{2k} \left( \frac{1}{m_1^2} q_{x0}^2 + \frac{1}{m_2^2} q_{y0}^2 \right)$$

(13)

and

$$q_{z2} = q_{z1}.$$  

(14)

Inserting Eqs. (4) and (11)–(14) in Eq. (8), taking into account that $\mathbf{e}_{y(1-1)} \parallel \mathbf{d}_i$ for $i=1,2$ holds, and performing the Fresnel approximation as discussed above the diffraction integral of the Bragg magnifier is obtained:

$$D_2(\mathbf{r}_2) = \int dq_{x0} dq_{y0} dq_{z0} \hat{D}_0(\mathbf{q}_{x0}, \mathbf{q}_{y0}, \mathbf{q}_{z0}) \hat{R}_1(\mathbf{q}_{x0}, \mathbf{q}_{y0}, \mathbf{q}_{z0}) \hat{R}_2(\mathbf{q}_{x0}, \mathbf{q}_{y0}, \mathbf{q}_{z0})$$

$$\times \exp \left\{ i \left[ -\frac{1}{m_1} q_{x0} r_{x2} - \frac{1}{m_2} q_{y0} r_{y2} + \frac{\mathbf{m}_1 r_{x2} - d_1}{2k} (q_{x0}^2 + q_{y0}^2) + \frac{\mathbf{m}_2 r_{y2} - d_2}{2k} (q_{y0}^2 + q_{z0}^2) \right] \right\}.$$  

(15)

As deviations from main beam directions are in the order of $q_{i} \approx 10^{-4}$ it is justified to use the standard coplanar approximation of diffraction theory: $\hat{R}_i(\mathbf{k}_{r-1}) = \hat{R}_i(q_{i0}/k)$. Equation (15) describes the most general case of imaging with the Bragg magnifier and can be simplified for realistic distances $d_i$ and magnification factors above $m_i=10$ to

$$D_2(\mathbf{r}_2) = \int dq_{x0} dq_{y0} dq_{z0} \hat{D}_0(\mathbf{q}_{x0}, \mathbf{q}_{y0}, \mathbf{q}_{z0}) \hat{R}_1(\mathbf{q}_{x0}, \mathbf{q}_{y0}, \mathbf{q}_{z0})$$

$$\times \exp \left\{ i \left[ -\frac{1}{m_1} q_{x0} r_{x2} - \frac{1}{m_2} q_{y0} r_{y2} + \frac{\mathbf{m}_1 r_{x2} - d_1}{2k} (q_{x0}^2 + q_{y0}^2) + \frac{\mathbf{m}_2 r_{y2} - d_2}{2k} (q_{y0}^2 + q_{z0}^2) \right] \right\}.$$  

(16)

For simplicity we will restrict the discussion in the following to one dimensional objects, thus neglecting the second reflection and the free space propagation after the first reflection. It is also convenient to rewrite the components of $\mathbf{r}_2$ to components of $\mathbf{r}_0$ defined in the original coordinate system $r_{i2} = -m_i r_{i0}$ and $r_{y0} = m_2 r_{x0} - d_2 = z$. Now the input amplitude can be written as $D_{0}(x,y) = D_{0}(x)$, the indices $x0$ can be omitted and Eq. (16) becomes a one-dimensional integral yielding

$$D_{out}(x) = \int dq \hat{D}_0(q) \hat{R} \left( \frac{q}{k} \right) e^{i(qx - z/2k^2)}$$

(17)

directly on the first analyzer surface [note the implicit dependence $z=z(x)$]. The restriction to one dimensional objects is the correct description of the imaging process for conventional DEI and a good approximation for vertical or horizontal lines of the image in the case of the Bragg Magnifier. Equation (17) was also motivated by Spal in Ref. 16.
D. Numerical simulation

In order to understand the imaging process we will use forward simulation in the sense that the diffraction integral (17) will be calculated numerically for several types of test amplitudes $D_0$ and the results will be discussed.

The numerical integration is done in the following way. For a given sample to analyzer distance $d_1$, Eq. (17) is merely the inverse Fourier transform of the function $\hat{D}_0(q)\hat{R}(q/k)\exp(-i\frac{z}{k}q^2)$. This can be conveniently computed with fast Fourier transform for several distances $d_1$. By displaying the resulting intensity distribution as a function of the back-projected position on sample $x$ and of the distance $z$, an “intensity landscape” is obtained (see Fig. 8). If just the intensity distribution along the analyzer surface is of interest linear interpolation to the position of the analyzer is applied to the intensity landscape [indicated by the black line in Fig. 8(b)]. We have used $2^{14}$ up to $2^{17}$ sample points in Fourier space in order to avoid numerical artifacts.

Different types of test amplitudes corresponding to increasingly realistic model samples will be discussed in the subsequent sections. We will start with a $\delta$ function as test amplitude in order to estimate the spatial resolution limit (as commonly done), demonstrate the influence of Bragg reflection on Fresnel diffraction at the example of a rectangular shaped amplitude and, finally, use a Gauss shaped model sample to investigate the dependence of the observable contrast on the sample to analyzer distance.

The reflection curve $\hat{R}(q/k)$ was calculated according to dynamical theory with the same parameters for all subsequent simulations: Si-224, $\sigma$ polarization, and a magnification factor of 40 at a photon energy of 8.048 keV, which is the first reflection of our experimental setup (see Fig. 9).

III. RESPONSE FUNCTION

Generally, a diffraction integral describing an imaging process can be analyzed by means of linear system theory. In this section we will work out the similarities and the limitations of the applicability of linear system theory to our case. In order to do so, we will analyze Eq. (17) in two steps. First we set the sample to analyzer distance $z$ to zero (i.e., neglecting the effects of Fresnel propagation). Using a $\delta$-shaped input amplitude, being the description of a single object point, and its well known Fourier transform $[\hat{D}_0(q) = \frac{1}{2\pi}]$ in Eq. (17) we obtain

$$R(x) = \int dq \hat{R}\left(\frac{q}{k}\right) e^{iqx}$$

which is exactly the inverse Fourier transform of the reflection curve. The function $R(x)$ is called influence function and its physical interpretation is as follows. A point source positioned directly on the crystal surface would imply a complex amplitude distribution after reflection described by the influence function (see Fig. 2).

Using again a $\delta$-shaped input amplitude, now taking Fresnel propagation to $z \neq 0$ into account, the response function (RF) for the Bragg magnifier is obtained

$$RF(x) = \int dq \hat{R}\left(\frac{q}{k}\right) e^{iqz-(z/2kq^2)}.$$  \hspace{1cm} (19)

The similarity to the amplitude spread function (ASF) in linear system theory is striking but misleading. In this theory the output amplitude $D_{\text{out}}$ is equal to the convolution of the input amplitude $D_0$ and the ASF: $D_{\text{out}} = D_0 \otimes \text{ASF}$. According to the convolution theorem, the Fourier transform of $D_{\text{out}}$ is the product of the individual Fourier transforms of $D_0$ and the ASF, respectively, yielding: $\hat{D}_{\text{out}} = \hat{D}_0 \cdot \text{ASF}$. But due to the dependence of $z(x)$ on $x$ formula (17) cannot be written as a simple convolution in direct space.

Figure 2 shows the numerically calculated response function for three different sample to analyzer distances and strongly emphasizes the necessity to take Fresnel propagation into account. Note that only the modulus of the RF is shown, not its phase distribution, so that the width of the first fringe does not necessarily correspond to the spatial resolution. This would only be true in the absence of any phase variations.

IV. RESOLUTION OF AN ABSORPTION OBJECT

The Sparrow criterion\textsuperscript{19} states that two image points are distinguishable if an intensity minimum exists between them. The criterion is therefore applicable for both coherent and incoherent illumination. The Sparrow criterion was applied in the following way. The amplitude in direct space of two image points separated by the distance $x_0$ is represented by
Obviously, the corresponding response functions of the two resolution limit. Consequently, the Sparrow criterion would state that the image therefore advantageous to construct instrumental realizations of the Bragg magnifier as compact as possible, to fully exploit these optimum conditions. The vertical axis of Fig. 3 shows that resolutions of few micrometers are easily accessible with the Bragg magnifier technique, and even resolutions well in the submicrometer regime (0.2–0.5 μm) are within reach if some care is taken to optimize the instrumental setup.

V. RESOLUTION OF A PHASE OBJECT

The spatial resolution limit in the case of phase objects can be dealt with by introducing a phase difference $\Delta \phi$ between the two object points $[i.e., D_0(x) = \delta(x) + \delta(x-x_0)e^{i\Delta \phi}]$. Let us first consider the case of a phase difference $\Delta \phi = \pi$. Obviously, the corresponding response functions of the two objects also differ in phase by a factor of $\pi$. Then the coherent superposition of the two always has a minimum, regardless of the distance between the two object points. Consequently, the Sparrow criterion would state that the image points are always separated, which would imply an infinite resolution limit.

$D_0(x) = \delta(x) + \delta(x-x_0)$. The resulting intensity distribution shows either one maximum (i.e., the Sparrow criterion is not fulfilled) or it shows two maxima corresponding to the two object points and a minimum between them. For the desired parameters (i.e., chosen reflection and sample to analyzer distance) the distance between the two object points $x_0$ was varied until the minimum separating the two maxima had contrast of 5% compared to the lower one of the two maxima.

Figure 3 shows the result of using the Sparrow criterion to determine the spatial resolution of the Bragg magnifier. It is obvious from the figure that the resolution limit varies by half an order of magnitude in the given interval of sample to analyzer distance (1 mm to 1 cm). According to these results, optimum resolution is predicted for the smallest distances. It is therefore advantageous to construct instrumental realizations of the Bragg magnifier as compact as possible, to fully exploit these optimum conditions. The vertical axis of Fig. 3 shows that resolutions of few micrometers are easily accessible with the Bragg magnifier technique, and even resolutions well in the submicrometer regime (0.2–0.5 μm) are within reach if some care is taken to optimize the instrumental setup.

VI. NUMERICAL EXAMPLES

A. Pure absorption objects

The effects of Fresnel diffraction on the propagation of a wave are commonly demonstrated at the example of diffraction at an edge. It is well known from light optics that oscillations, called Fresnel fringes, occur in the geometrically il-
The surprising result is that Fresnel fringes are strongly attenuated by the reflection. For explanation, consider that fast oscillations in direct space (i.e., Fresnel fringes) correspond to high frequencies in Fourier space. High frequencies in Fourier space are suppressed by the reflection curve and therefore cannot pass the analyzer crystal. Therefore, the observable intensity distribution is smoothed, thus eliminating parts of the fringe systems.

**B. Phase objects**

The results of the preceding sections will now be validated for a realistic test sample. In order to facilitate easy interpretation a Gauss shaped test sample was chosen. The input amplitude in direct space \( D_0(x) \) was calculated according to formula (1) with the complex refractive index of amorphous carbon (modeling biological samples). The numerically calculated Fourier transform of the input amplitude \( D_0(q) \) was used to compute the diffraction integral (17).

The Gauss function of the test sample (indicated by the shaded area in Fig. 7) had a variance of 1 \( \mu m \) and a thickness of 5 \( \mu m \), thus providing an (intensity) absorption contrast of about 0.4\%, a maximum phase variation of about \( \pi/2 \) and maximum phase variation of about 0.6 \( \mu rad \) (i.e., ten times the minimum detectable phase variation estimated above).
Figure 7 shows the calculated intensity distribution along the analyzer surface in the medium sample to analyzer distance $z = 10$ mm for the case of Fresnel propagation (in-line holography; dashed line) and after the Si-224 reflection with a magnification factor of 40 (imaging with the Bragg magnifier; solid line).

As expected the intensity distribution without reflection is proportional to the Laplacian of the phase\textsuperscript{21} whereas with reflection it is roughly proportional to the gradient of the phase\textsuperscript{8,22} resulting in the typical dark-bright contrast of analyzer based imaging. For the given parameters the contrast of imaging with the Bragg magnifier is about twice as strong as for in-line holography. Furthermore, paying special attention to the slopes of the intensity distributions, smaller phase variations are detectable after reflection indicating that analyzer-based imaging is more sensitive to phase variations than in-line holography and thus more sensitive to density variations present in the sample.

We conclude this section with a comparison of the intensity landscapes calculated for free space propagation and after reflection (Fig. 8), using the same parameters as in Fig. 7. The focussing behavior visible in Fig. 8(a) is due to the special shape of the test sample which roughly corresponds to refractive x-ray lenses. The typical dark-bright contrast for analyzer based imaging [Fig. 8(b)] is preserved during the propagation, underlining the small influence of Fresnel diffraction. Realizing that the strongest dark-bright contrast at a distance of 100 mm in Fig. 8(b) is the desired contrast, it can even be stated that the attenuation of Fresnel fringes after reflection holds true for the case of phase objects.

Comparing both imaging techniques it can be stated that the contrast of imaging with the Bragg magnifier is comparable with or even at small distances superior to the contrast of in-line holography. It is also striking that the contrast as a function of distance is approximately constant, thus allowing one to reduce sample to analyzer distance in order to improve the spatial resolution (as discussed above) without losing contrast. Furthermore, by comparing Figs. 8(a) and 8(b) it is striking that the divergence is reduced for the case with reflection, thus making the resolution dependence on distance for the Bragg magnifier superior to in-line holography.

VII. EXPERIMENTAL EXAMPLE

The experiment was carried out at the ID-02-01 beamline (“BAMLine”) of the Bessy Synchrotron, Berlin. The x-ray source was a 7 T wavelength shifter. The imaging system was implemented in a very compact setup (the “Bragg magnifier box,” Fig. 9) and was tested in the laboratory before being transferred to the beamline as a turnkey instrument. In Fig. 9 the x-ray beam enters from the right through a system of slits and then hits the sample, which is mounted on a vertical rotation axis on top of a translation stage. After transmission through the sample, the beam is diffracted in two mutually perpendicular directions: vertically by the first analyzer crystal (Si-224 reflection) and horizontally by the second analyzer (Si-004 reflection). At the x-ray energy used (Cu-K\textalpha\textsuperscript{a}, $\lambda = 1.54$ Å, from a double-crystal monochromator), the scattering angle of the first reflection was close to 90° — a geometric precondition for realizing a short distance between the two analyzer crystals. Both crystals were asymmetrically cut, with asymmetries chosen in such a way that the magnification factors in both image dimensions were 40. The tilt angles of both analyzers were adjusted to realize shear-free imaging conditions, as verified with the help of a rectangular grid test object.

After being reflected twice, the (laterally expanded) beam left the instrument through the front-side circular opening, which was used to mount a CCD camera. The detector was a commercial Bruker-AXS Smart Apex 2 camera with 4096\textsuperscript{2} pixels and a nominal pixel size of 15 $\mu$m. It provided several binning modes, of which 1 $\times$ 1 binning (i.e., no binning) was used for two-dimensional imaging (effective pixel size 0.375 $\mu$m), and 2 $\times$ 2 binning was used for the tomographic scans (effective pixel size 0.75 $\mu$m) to speed up acquisition. The setup had a total field of view of 1.5 mm. Tomographic scans were taken by recording series of up to 720 magnified projection images upon sample rotation around the vertical axis.

FIG. 8. (Color online) Comparison of the intensity landscapes in case of free space propagation (a) and after reflection (b). The test sample was Gauss shaped amorphous carbon, see Fig. 7. The observable intensity is calculated in dependence on the backprojected position on sample (horizontal axis) and on the distance between sample and analyzer (vertical axis). The line in (b) indicates the position of the analyzer surface of Fig. 7.
Figure 10 shows a magnified two-dimensional projection image of a spider leg, used as a model object. The analyzers were tuned to the flank of their rocking curve to yield maximum phase contrast, as obvious from the characteristic double-contrast (dark-bright) visible at each of the lateral features ("hair") of the spider leg. While the use of phase contrast enhances image contrast and improves spatial resolution (see Sec. V), it can, in principle, pose a problem for three-dimensional tomographic reconstruction. Conventional algorithms and available software for 3D reconstruction are usually based on pure absorption contrast. Application to series of projection images showing strong phase contrast, as in Fig. 10, is therefore considered a purely tentative procedure. However, effects of dispersion and divergence reduce the visibility of Kato and Fresnel fringes in the experimental images, thus reducing the quantitative information contents in the images but improving the qualitative resemblance between sample and image. For the simple algorithm used here for tentative 3D reconstruction this even has the beneficial effect of reducing artefacts during reconstruction. The result in Fig. 11 demonstrates that a very reasonable 3D representation of the spider leg can be obtained, giving a clear image of both the overall external shape and the inner structure of the object.

Further optimization of the data evaluation and image reconstruction procedure will be performed by developing a dedicated tomographic reconstruction algorithm for phase contrast imaging. An approach based on interleaved sample rotation and analyzer rocking scans has already been taken.

Moreover, we are presently performing more detailed studies on the quantitative influence of the effects of beam dispersion and divergence in the experimental images.

FIG. 9. (Color online) Technical sketch of the Bragg magnifier. The path of x-rays (incident from the right) is indicated by bright lines, the position of the sample by the darker line. The ring near the end of the x-ray path indicates the position of the CCD camera. For reasons of clarity some components of the instrument have been omitted from the picture.

FIG. 10. Experimental projection image of a spider leg acquired at a working point on the left flank of the first analyzer reflection curve. Note the dark-bright double contrast at the vertical structures ("hair"), which is a clear evidence of phase contrast. Also note that this image is less strongly affected by Fresnel and Kato fringes than might be expected from theory, due to both the complex inner structure of the object and remaining divergence and dispersion of the incident beam.

FIG. 11. (Color online) Three-dimensional reconstruction of phase contrast tomographic data of the spider leg. Data evaluation was performed by applying the DEI algorithm (Ref. 5) at each individual sample rotation position prior to reconstruction. The cube in the lower right corner has a edge length of 100 μm.
dissipation and dispersion on image quality. The approach is based on incoherent superposition of several partial images generated by the different components of the wave field. Preliminary results show that under our experimental conditions dispersion is the dominating influence reducing the expected contrast by about a factor of 2, but preserving the qualitative phase contrast distribution.

VIII. DISCUSSION

The theoretical framework presented above covers wave propagation over the entire spatial range from sample to detector. Experimental results show that magnification in both image dimensions has been achieved independently, with no additional shear between the x and y dimensions (see Refs. 7 and 11). This was one main goal in instrument design, and indicates that the two analyzer crystals are well aligned within two mutally perpendicular diffraction planes. Contrast simulations for the case of a simplified one-dimensional object and a single analyzer crystal show the influence of interference phenomena related to propagation in space and to diffraction. Up to now these effects were not taken fully into account in the literature, although they are quite essential for the discussion of spatial resolution. These simulations demonstrate that phase sensitivity of “Bragg magnification” is superior to that of conventional in-line holography. This advantage holds in particular for comparatively short distances between sample and analyzer crystals. Regarding resolution there is a trade-off in view of angular acceptance of the analyzer crystals: large angular acceptance (low index reflections, comparatively long wavelengths) results in a small half width of the influence function (good spatial resolution in diffraction), but also in a low phase sensitivity and a considerable spread of the signal during propagation. Conversely, a small angle of acceptance leads to a more extended influence function but also to higher phase sensitivity and a lower spread of the signal during propagation. Therefore, the Bragg magnifier setup presented here was constructed with the following compromise in mind: short sample to analyzer distances and medium acceptance angles. This gives an extended range of good spatial resolution, i.e., allows for large fields of view. Using magnification factors of 40 and above the field of view after magnification is well adapted to current high-performance CCD detectors with spatial resolutions in the range of few ten micrometers.

The calculations given above were performed for the case of incident monochromatic plane waves. The influence of additional dispersion and divergence of the incoming beam on contrast will be the subject of a forthcoming paper. Preliminary results show that as long as their combined effect (angular spread due to divergence and dispersion) does not considerably exceed the angular acceptance of the analyzer, the phase contrast features are essentially preserved, even though contrast is quantitatively reduced as compared to the plane wave case. Propagation contrast is slightly less sensitive to divergence. Even in the case of predominance of propagation contrast the use of magnifier crystals proves useful as the acceptance angle cuts a part of the interference pattern of propagation contrast of a single object and elimi-

nates far reaching interference phenomena. In the given experimental case the analyzer acceptance angles were roughly comparable to the angular width corresponding to the finite bandwidth. In other words, nearly the whole radiation impinging on the sample contributed to image formation. This further contributed to the efficiency of the entire imaging process, in addition to the fact that thanks to magnification a comparatively thick luminescence layer with high x-ray absorption efficiency could be used in the CCD camera, which also allowed for comparatively short exposure times at a good pixel resolution (0.75 or 0.375 µm at the sample plane) and a high dynamic range.

IX. CONCLUSION

In conclusion, we have established a theory of the process of image formation in analyzer-based magnified x-ray imaging. The theory takes into account the processes of both Fresnel propagation and Bragg reflection.

Numerical simulations were performed based on the above theory. A set of numerical model objects was used to analyze the spatial resolution achievable with the imaging setup. One result from simulations is that the influences of simultaneously occurring Fresnel and Kato fringes damp each other, thus yielding a better overall spatial resolution than expected from a naive theory. The simulations further show that spatial resolution is optimal for a very compact instrumental setup.

Comparison of different model objects shows that the achievable resolution is indeed superior for phase contrast as compared to pure absorption objects. This further underlines the attractiveness of exploiting phase contrast mechanisms for microstructural investigations.

In view of the above findings, the experimental instrument (“Bragg magnifier box”) was designed as compact as possible, realizing a very short distance between the two analyzer crystals for optimum spatial resolution. Two dimensional image magnification by factors of 40 was achieved, with pixel sizes of 0.75 and 0.375 µm.

Simultaneously, strong phase contrast was achieved, as evidenced, e.g., by double-contrast features in projection images. The series of magnified radiographic images proved suitable for 3D tomographic reconstruction using conventional (absorption-based) reconstruction software, yielding 3D data sets with submicrometer voxel sizes which give access to the full external and internal structure of the object investigated.

Future developments will include a full 3D reconstruction algorithm simultaneously also fully taking into account phase contrast. Combined tomographic and DEI scans will prove decisive for quantitative phase analysis in two- and three-dimensional imaging.

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